2015
ARO
IN REVIEW

U.S. Army Research Laboratory (ARL)
U.S. Army Research Office (ARO)
P.O. Box 12211
Research Triangle Park, NC 27709-2211

ARO IN REVIEW 2015

TABLE OF CONTENTS

CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY

This report is intended to be a single-source document describing the research programs of the U.S. Army Research Laboratory's Army Research Office (ARO) for fiscal year 2015 (FY15; 1 Oct 2014 through 30 Sep 2015). This report provides:

- A brief review of the strategy employed to guide ARO research investments and noteworthy issues affecting the implementation of that strategy
- Statistics regarding basic research funding (*i.e.*, "6.1" funding) and program proposal activity
- Research trends and accomplishments of the individual ARO scientific divisions

I. ARO MISSION

The mission of ARO, as part of the U.S. Army Research Laboratory (ARL), is to execute the Army's extramural basic research program in the following disciplines: chemical sciences, computing sciences, electronics, life sciences, materials science, mathematical sciences, mechanical sciences, network sciences, and physics. The goal of this basic research is to drive scientific discoveries that will provide the Army with significant advances in operational capabilities through high-risk, high pay-off research opportunities, primarily with universities, but also with large and small businesses. ARO ensures that this research supports all of the ARL Science and Technology (S&T) Campaigns, and that the results of these efforts are transitioned to the Army research and development community for the pursuit of long-term technological advances for the Army.

II. ARO STRATEGY AND FUNCTION

ARO's mission represents the most long-range Army view for changes in its technology, with system applications often 20-30 years away. ARO pursues a long-range investment strategy designed to maintain the Army's overmatch capability in the expanding range of present and future operational capabilities. ARO competitively selects and funds basic research proposals from educational institutions, nonprofit organizations, and private industry. ARO executes its mission through conduct of an aggressive basic science research program on behalf of the Army to create cutting-edge scientific discoveries and the general store of scientific knowledge that is required to develop and improve weapons systems for land force dominance. The ARO research portfolio consists principally of extramural academic research efforts consisting of single investigator efforts, university-affiliated research centers, and specially tailored outreach programs. Each program has its own objectives and set of advantages as described further in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

ARL has eight S&T Campaigns (listed in Section III-B), including an extramural basic research campaign that ARO leads. ARO supports research that will lead to new discoveries and increased understanding of the physical, engineering, and information sciences as they relate to long-term national security needs, in addition to the other seven ARL Campaigns.

The ARO strategy and programs, as part of the ARL Extramural Basic Research Campaign, are formulated in concert with the other ARL S&T Campaigns, the Research, Development and Engineering Command's (RDECOM's) Research, Development and Engineering Centers (RDECs), the Army Medical Research and Materiel Command (MRMC), the Army Corps of Engineers, and the Army Research Institute for the Behavioral and Social Sciences. ARO programs and research areas are intimately aligned with, and fully supportive of, the research priorities set within the DoD Quadrennial Defense Review (QDR), the DoD Strategic Basic Research Plan, the Assistant Secretary of Defense for Research and Engineering [ASD(R&E)] S&T Priorities, the Army S&T Master Plan, the Training and Doctrine Command (TRADOC) Army Capabilities Integration Center's Integrated S&T Lines of Effort, the TRADOC Army Warfighting Challenges, and the Assistant Secretary of the Army for Acquisition, Logistics, and Technology [ASA(ALT)] Special Focus Areas.

ARO serves the following functions in pursuit of its mission.

- Execute an integrated, balanced extramural basic research program
- Create and guide the discovery and application of novel scientific phenomena leading to leap-ahead technologies for the Army
- Drive the application of science to generate new or improved solutions to existing needs
- Accelerate research results transition to applications in all stages of the research and development cycle
- Strengthen the research infrastructures of academic, industrial, and nonprofit laboratories that support the Army
- Focus on research topics that support technologies vital to the Army's future force, combating terrorism and new emerging threats
- Leverage S&T of other defense and government laboratories, academia and industry, and organizations of our allies
- Foster training for scientists and engineers in the scientific disciplines critical to Army needs
- Actively seek creative approaches to enhance the diversity and capabilities of future U.S. research programs by enhancing education and research programs at historically black colleges and universities, and minority-serving institutions

III. IMPLEMENTING ARO STRATEGY

ARO employs multiple programs, initiatives, and investment strategies to fulfill its mission. A snapshot of the ARO research programs is provided in this section, and each program is described further in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

A. Program Snapshot

The research programs managed by ARO range from single investigator research to multidisciplinary/multi-investigator initiatives. A typical basic research grant within a program may provide funding for a few years, while in other programs, such as research centers affiliated with particular universities, a group of investigators may receive funding for many years to pursue novel research concepts. The programs for the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) are aimed at providing infrastructure and incentives to improve the diversity of U.S. basic research programs (see CHAPTER 2-IX). In addition to supporting the education of graduate students through basic research grants, the National Defense Science and Engineering Graduate (NDSEG) fellowship program is another mechanism through which ARO fosters the training of a highly-educated workforce skilled in DoD and Army-relevant research, which is critical for the future of the nation (see CHAPTER 2-X). ARO also has extensive programs in outreach to pre-graduate education to encourage and enable the next generation of scientists (see CHAPTER 2-XI). In addition, ARO guides the transition of basic research discoveries and advances to the appropriate applied-research and advanced-development organizations. ARO is actively engaged in speeding the transition of discovery into systems, in part through involvement in the development of topics and the management of projects in the Small Business Innovation Research (SBIR) and Small Business Technology Transfer (STTR) programs (see CHAPTER 2-VIII).

B. Coordination for Program Development and Monitoring

The research programs and initiatives that compose ARO's extramural research program are formulated through an ongoing and active collaboration with a variety of Federal research organizations, including the:

- ARL S&T Campaigns (in addition to the ARL Extramural Basic Research Campaign)
  - Computational Sciences Campaign
  - Materials Research Campaign
  - Sciences-for-Maneuver Campaign
  - Information Sciences Campaign
  - Sciences for Lethality-and-Protection Campaign
  - Human Sciences Campaign
  - Assessment and Analysis Campaign
- ARL Directorates:
  - Computational and Information Sciences Directorate (ARL-CISD)
  - Human Research and Engineering Directorate (ARL-HRED)
  - Sensors and Electron Devices Directorate (ARL-SEDD)
  - Survivability/Lethality Analysis Directorate (ARL-SLAD)
  - Vehicle Technology Directorate (ARL-VTD)
  - Weapons and Materials Research Directorate (ARL-WMRD)
- RDECOM's RDECs
- Army Medical Research and Materiel Command (MRMC)
- Army Corps of Engineers
- Army Research Institute for the Behavioral and Social Sciences
- Army Training and Doctrine Command (TRADOC)

ARO's extramural research program provides foundational discoveries in support of the ARL S&T Campaign Plans. While the ARL Directorates and the RDECOM Centers are the primary users of the results of the ARO research program, ARO also supports research of interest to the Army Corps of Engineers, MRMC, other Army Commands, and DoD agencies. Coordination and monitoring of the ARO extramural program by the ARL Directorates, RDECs, and other Army laboratories ensures a highly productive and cost-effective Army research effort. The University Affiliated Research Centers (UARCs) and Multidisciplinary University Research Initiative (MURI) centers benefit from the expertise and guidance provided by the ARL Directorates, RDECs, and other DoD, academic, and industry representatives who serve on evaluation panels for each UARC.

The ARO-managed OSD research programs include the University Research Initiative (URI) programs, and the Research and Educational Program (REP) for HBCU/MIs. These programs fall under the executive oversight of the Defense Basic Research Advisory Group. This group is led by the ASD(R&E) Director for Research, representatives from the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the Defense Advanced Research Projects Agency (DARPA), ARO, and ASAALT.

IV. REVIEW AND EVALUATION

The ARO Directorates, Divisions, and Programs are evaluated by a wide range of internal (Army) and external (Academic, other Government) reviews, such as the biennial ARO Division Reviews. For additional information regarding these review processes, the reader is encouraged to refer to the corresponding presentations and reports from each review (not included here).

V. ARO ORGANIZATIONAL STRUCTURE

The organizational structure of ARO mirrors the departmental structure found in many research universities. ARO's scientific divisions are aligned to a specific scientific discipline (*e.g.*, chemical sciences), and supported by the Operations Directorate (see FIGURE 1).

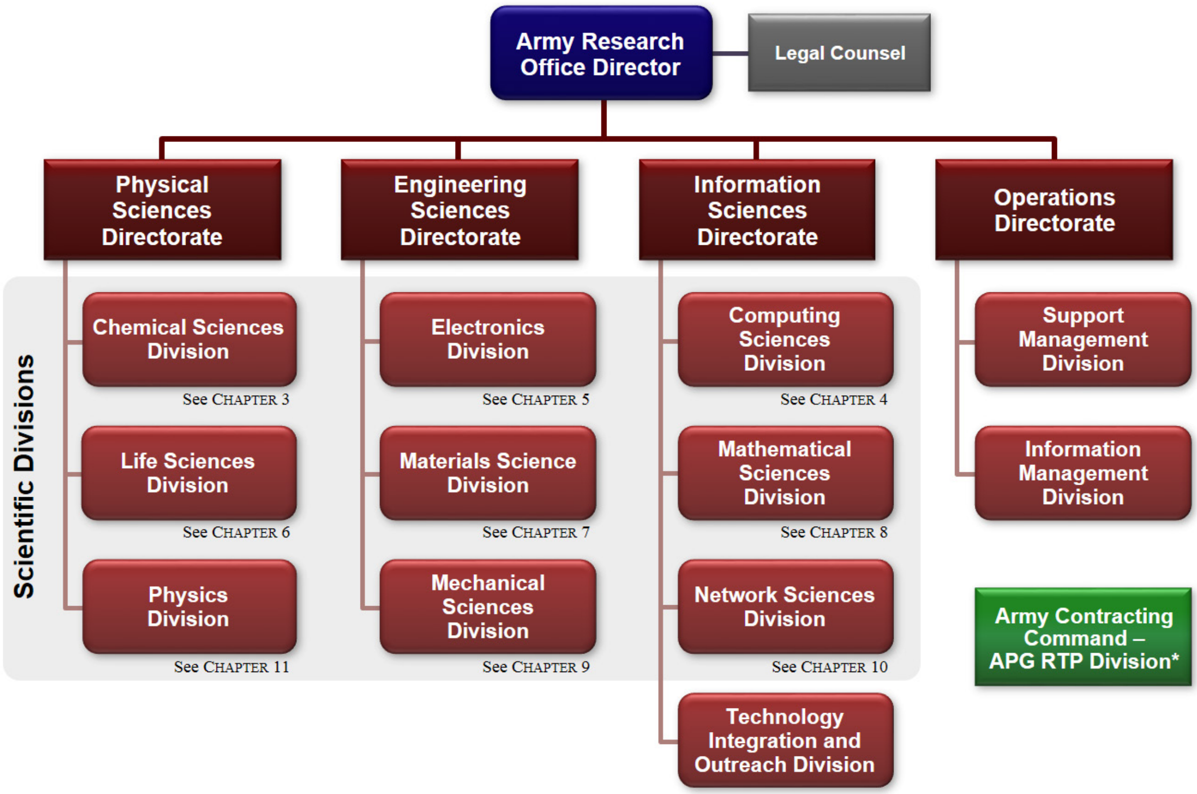

FIGURE 1

ARO Organizational Structure. ARO's scientific divisions fall under the Physical Sciences, Engineering Sciences, and Information Sciences Directorates. Each scientific division has its own vision and research objectives, as described further in CHAPTERS 3-11. *The Army Contracting Command – Army Proving Ground (APG), Research Triangle Park (RTP) Division executes the contracting needs for ARO-funded research; however, as part of the Army Contracting Command (*i.e.*, not ARL), it also performs contracting activities throughout RDECOM.

VI. ARO DIRECTOR'S OFFICE STAFF

Dr. David Skatrud
ARO Director
ARL Deputy Director for Basic Science

Dr. Stephen Lee
Chief Scientist

LTC Thomas "Bull" Holland
Military Deputy

Mr. Edward Beauchamp, Esq.
Legal Counsel

Mr. Richard Freed
Associate Director for Business and Research Administration

Dr. Brian Ashford
Special Assistant to the Director

Ms. Tish Torgerson
Program Administrative Specialist

CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES

As described in the previous chapter, ARO pursues a variety of investment strategies to meet its mission as the Army's lead extramural basic research agency in chemical sciences, computing sciences, electronics, life sciences, materials science, mathematical sciences, mechanical sciences, network sciences, and physics. ARO implements these investment strategies through research programs and initiatives that have unique objectives, eligibility requirements, and receive funding from a variety of DoD sources. This chapter describes the visions, objectives, and funding sources of these programs, which compose the overall ARO extramural research program.

The selection of research topics, proposal evaluation, and project monitoring are organized within ARO Divisions according to scientific discipline (refer to the organizational chart presented in CHAPTER 1). ARO's Divisions are aligned with these disciplines, each with its own vision and research objectives, as detailed in CHAPTERS 3-11. Each Division identifies topics that are included in the broad agency announcement (BAA). Researchers are encouraged to submit white papers and proposals in areas that support the Division's objectives. It is noted that the ARO Divisions are not confined to only funding research in the academic departments that align with the Division names. The Divisions have the flexibility to find and fund the most promising research to advance their mission regardless of the academic department pursuing a particular research idea.

I. OVERVIEW OF PROGRAM FUNDING SOURCES

ARO oversees and participates in the topic generation, proposal solicitation, evaluation, and grant-monitoring activities of programs funded through a variety of DoD agencies, as discussed in the following subsections.

A. Army Funding

The Army funds the majority of the extramural basic research programs managed by ARO. These programs are indicated below and are described in more detail later in this chapter.

- The Core (BH57) Research Program, funded through basic research "BH57" funds (see Section II).
- The University Research Initiative (URI), which includes these component programs:
  - Multidisciplinary University Research Initiative (MURI) program (see Section III)
  - Presidential Early Career Awards for Scientists and Engineers (PECASE; see Section IV)
  - Defense University Research Instrumentation Program (DURIP; see Section V)
- Two University Affiliated Research Centers (UARCs; see Section VI)

ARO coordinates with the Office of the Secretary of Defense (OSD) in managing the URI programs and also manages the Army's Small Business Technology Transfer (STTR) program (see Section VIII).

B. Office of the Secretary of Defense (OSD) Funding

The funds for a variety of programs managed or supported by ARO are provided by OSD.

- Research and Educational Program (REP) for Historically Black Colleges and Universities and Minority Institutions (HBCU/MI; see Section IX)
- National Defense Science and Engineering Graduate (NDSEG) Fellowships (see Section X)
- Youth Science Activities (see Section XI)

These activities are mandated by DoD's Chief Technology Office, the Assistant Secretary of Defense for Research and Engineering ASD(R&E). Each of these OSD-funded programs has a unique focus and/or a unique target audience. ARO has been designated by ASD(R&E) as the lead agency for the implementation of REP for HBCU/MI activities on behalf of the three Services. OSD oversees ARO management of the Army-funded URI and its component programs (MURI, PECASE, and DURIP).

C. Other Funding Sources

In addition to the Army- and OSD-funded programs described earlier in this section, ARO leverages funds from other DoD sources (*e.g.*, Defense Advanced Research Projects Agency [DARPA]) to support a variety of external programs with specific research focuses. These joint programs have objectives consistent with the strategies of the corresponding ARO Program. Due to the unique nature of these cooperative efforts, each externally-funded effort is discussed within the chapter of the aligned scientific Division (see CHAPTERS 3-11).

II. ARO CORE (BH57) RESEARCH PROGRAM

ARO's Core Research Program is funded with Army basic research "BH57" funds and represents the primary basic research funding provided to ARO by the Army. Within this program and its ongoing BAA, research proposals are sought from educational institutions, nonprofit organizations, and commercial organizations for basic research in electronics, physics, and the chemical, computing, life, materials, mathematical, mechanical, and network sciences. The goal of this program is to utilize world-class and worldwide academic expertise to discover and exploit novel scientific opportunities, primarily at universities, to provide the current and future force with critical new or enhanced capabilities.

ARO Core Research Program activities fall under five categories, discussed in the following subsections: (a) Single Investigator awards, (b) Short Term Innovative Research efforts, (c) Young Investigator Program, (d) support for conferences, workshops, and symposia, and (e) special programs. ARO's Core (BH57) Research Program represents the principal mission of ARO and is where the majority of the Army funds are used. A summary of the Core (BH57) Research Program budget is presented in Section XIII.

A. Single Investigator (SI) Program

The goal of the SI program is to pursue the most innovative, high-risk, and high-payoff ideas in basic research. Research proposals within the SI Program are received throughout the year in a continuously-open, worldwide BAA solicitation. This program focuses on basic research efforts by one or two faculty members along with supporting graduate students and/or postdoctoral researchers and is typically a three-year grant.

B. Short Term Innovative Research (STIR) Program

The objective of the STIR Program is to explore high-risk initial proof-of-concept ideas within a nine-month timeframe. Research proposals are sought from educational institutions, nonprofit organizations, or private industry. If a STIR effort's results are promising, the investigator may be encouraged to submit a proposal to be evaluated for potential longer-term funding options, such as an SI award.

C. Young Investigator Program (YIP)

The objective of the YIP is to attract outstanding young university faculty to Army-relevant research questions, to support their research, and to encourage their teaching and research careers. Outstanding YIP projects may be considered for the prestigious PECASE award (see Section IV).

D. Conferences, Workshops, and Symposia Support Program

The ARO Core Program also provides funding for organizing and facilitating scientific and technical conferences, workshops, and symposia. This program provides a method for conducting scientific and technical meetings that facilitate the exchange of scientific information relevant to the long-term basic research interests of the Army and help define research needs, thrusts, opportunities, and innovation. In particular, workshops are a key mechanism ARO uses to identify new research areas with the greatest opportunities for scientific breakthroughs that will revolutionize future Army capabilities.

E. Special Programs

Although the ARO SI, STIR, YIP, and conference-support programs constitute the primary use of BH57 funds, the ARO Core Research Program also supports a variety of special programs. These special programs include matching funds applied to the ARO Core-funded HBCU/MI program, and also the Army-supported High School Apprenticeship Program (HSAP) and Undergraduate Research Apprenticeship Program (URAP), which are part of the Youth Science Activities (see Section XI).

III. MULTIDISCIPLINARY UNIVERSITY RESEARCH INITIATIVE (MURI)

As described in Section I: *Overview of Program Funding Sources*, the MURI Program is part of the University Research Initiative (URI) and supports research teams whose research efforts intersect more than one traditional discipline. A multidisciplinary team effort can accelerate research progress in areas particularly suited to this approach by cross-fertilization of ideas, can hasten the transition of basic research findings to practical applications, and can help to train students in science and/or engineering in areas of importance to DoD.

In contrast with ARO Core program SI research projects, MURI projects support centers whose efforts require a large and highly collaborative mutidisciplinary research effort. They are typically funded at $1.25 million per year for three years with an option for two additional years. These efforts are expected to enable more rapid research and development (R&D) breakthroughs and to promote eventual transition to Army applications.

Management oversight of the MURI program comes from the Basic Research Office of ASD(R&E) to the Service Research Offices (OXRs), where OXR program managers (PM) oversee the MURI projects. The OXRs include ARO, the Air force Office of Scientific Research (AFOSR), and the Office of Naval Research (ONR). OXR PMs have significant flexibility and discretion in how the individual projects are monitored and managed, while ASD(R&E) defends the program to higher levels in OSD and has responsibility for overall program direction and oversight. Selection of Army research topics and the eventual awards are reviewed and approved by ASD(R&E) under a formal acquisition process.

Eight MURI projects were selected for funding and began in FY15. These projects are based on proposals submitted to the FY15 MURI topic BAA, which was released in late FY14. Each new-start project, lead investigator, and lead performing organization are listed here, immediately below the corresponding MURI topic, topic authors / program managers, and the ARO Division responsible for monitoring the project. A description of each of these projects can be found in the corresponding Division's chapter, based on the topic's lead author.

- Topic: *Emulating the Principles of Impulsive Biological Force Generation*; Topic Authors: Dr. Samuel Stanton, Mechanical Sciences and Dr. Robert Kokoska, Life Sciences

  Project Selected: *Evolutionary Mechanics of Impulsive Biological Systems: Guiding Scalable Synthetic Design*; Professor Sheila Patek, Duke University

- Topic: *Exploiting Nitrogen Vacancy Diamonds For Manipulation Of Biological Transduction*; Topic Authors: Dr. Frederick Gregory, Life Sciences and Dr. Paul Baker, Physics
  Project Selected*: Imaging and Control of Biological Transduction using NV-Diamond*; Professor Ronald Walsworth, Harvard University
- Topic: *Noncommutativity in Interdependent Multimodal Data Analysis*; Topic Authors: Dr. Liyi Dai, Computing Sciences and Dr. T.R. Govindan, Physics
  Project Selected: *Adaptive Exploitation of Noncommutative Multimodal Information Structure*; Professor Negar Kiyavash, University of Illinois at Urbana-Champaign
- Topic: *Multi-Scale Response for Adaptive Chemical and Material Systems*; Topic Authors: Dr. Dawanne Poree, Chemical Sciences and Dr. John Prater, Materials Science
  Project Selected: *Specifically Triggerable Multi-Scale Responses in Organized Assemblies*; Professor Sankaran Thayumanavan, University of Massachusetts-Amherst
- Topic: *New Regimes in Quantum Optics*; Topic Authors: Dr. T.R. Govindan, Physics and Dr. Joe Qiu, Electronics
  Project Selected: *Engineering Exotic States of Light with Superconducting Circuits*; Professor Andrew Houck, Princeton University
- Topic: *Fractional Order Methods for Sharp Interface Flows*; Topic Author: Dr. Joe Myers, Mathematical Sciences
  Project Selected: *Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics and Applications*; Professor George Karniadakis, Brown University
- Topic: *2-Dimensional Organic Polymers*; Topic Authors: Dr. Pani Varanasi, Materials Science and Dr. Dawanne Poree, Chemical Sciences
  Project Selected: *Center for Advanced 2D Networks*; Professor William Dichtel, Cornell University
- Topic: *Network Science of Teams*; Topic Author: Dr. Edward Palazzolo, Network Sciences
  Project Selected: *QUANTA: Quantitative Network-based Models of Adaptive Team Behavior*; Dr. Ambuj Singh, University of California - Santa Barbara

The following topics were published in FY15 and constitute the ARO portion of the FY16 MURI BAA. The topic titles, topic author(s), and corresponding ARO Division(s) are listed below.

- *Sequence-Defined Synthetic Polymers Enabled by Engineered Translation Machinery*; Dr. Dawanne Poree, Chemical Sciences and Dr. Stephanie McElhinny, Life Sciences
- *Discovering Hidden Phases with Electromagnetic Excitation*; Dr. Marc Ulrich, Physics and Dr. Pani Varanasi, Materials Science
- *Modeling and Analysis of Multisensory Neural Information Processing for Direct Brain-Computer Communications*; Dr. Liyi Dai, Computing Sciences and Dr. Frederick Gregory, Life Sciences
- *Modular Quantum Systems*; Dr. T.R. Govindan and Dr. Tatjana Curcic, AFOSR
- *Spin Textures and Dynamics Induced by Spin-Orbit Coupling*; Dr. Joe Qui, Electronics, Dr. John Prater, Materials Science and Dr. Marc Ulrich, Physics
- *Defining Expertise by Discovering the Underlying Neural Mechanisms of Skill Learning*; Dr. Frederick Gregory, Life Sciences and Virginia Pasour, Mathematical Sciences
- *Media Analytics for Developing & Testing Theories of Social Structure & Interaction*; Dr. Purush Iyer, Network Sciences and Dr. Micheline Strand, Life Sciences
- *Fundamental Properties of Energy Flow and Partitioning at Sub-nanoscale Interfaces*; Dr. Robert Mantz, Chemical Sciences and Dr. Ralph Anthenien, Mechanical Sciences

IV. PRESIDENTIAL EARLY CAREER AWARD FOR SCIENTISTS AND ENGINEERS (PECASE)

The PECASE program, also part of the URI program, attracts outstanding young university faculty members, supporting their research, and encouraging their teaching and research careers. PECASE awards are the highest honor bestowed by the Army to outstanding scientists and engineers beginning their independent research careers. Each award averages $200K/year for five years. PECASE awards are based in part on two important criteria: (i) innovative research at the frontiers of science and technology (S&T) that is relevant to the mission of the sponsoring organization or agency, and (ii) community service demonstrated through scientific leadership, education, and community outreach.

The PECASE winners for each calendar year are typically announced by the White House at the end of the fiscal year. However, the PECASE recipients for the 2013, 2014, and 2015 competitions had not yet been announced by the close of FY15.

V. DEFENSE UNIVERSITY RESEARCH INSTRUMENTATION PROGRAM (DURIP)

DURIP, also part of the URI program, supports the purchase of state-of-the-art equipment that augments current university capabilities or develops new university capabilities to perform cutting-edge defense research. DURIP meets a critical need by enabling university researchers to purchase scientific equipment costing $50K or more to conduct DoD-relevant research. In FY15, the Army awarded 70 grants at $13,997,187 total, with an average award of $213K.

VI. UNIVERSITY AFFILIATED RESEARCH CENTERS (UARCS)

The University Affiliated Research Centers (UARCs) are strategic DoD-established research organizations at universities. The UARCs were formally established in May 1996 by ASD(R&E) in order to advance DoD long-term goals by pursuing leading-edge basic research and to maintain core competencies in specific domains unique to each UARC, for the benefit of DoD components and agencies. One DoD Service or Agency is formally designated by ASD(R&E) to be the primary sponsor for each UARC. The primary sponsor ensures DoD UARC management policies and procedures are properly implemented. Collaborations among UARCs and the educational and research resources available at the associated universities can enhance each UARC's ability to meet the long-term goals of DoD. ARO is the primary sponsor for the two UARCs listed below.

- The Institute for Soldier Nanotechnologies (ISN), located at the Massachusetts Institute of Technology (MIT). The ISN is discussed further in CHAPTER 3: CHEMICAL SCIENCES DIVISION.
- The Institute for Collaborative Biotechnologies (ICB), located at the University of California - Santa Barbara, with academic partners at MIT and the California Institute of Technology. The ICB is discussed further in CHAPTER 6: LIFE SCIENCES DIVISION.

VII. MINERVA RESEARCH INITIATIVE (MRI)

The Minerva Research Initiative (MRI) is a DoD-sponsored, university-based social science basic research program initiated by the Secretary of Defense and focuses on areas of strategic importance to U.S. national security policy. It seeks to increase the intellectual capital in the social sciences and improve DoD's ability to address future challenges and build bridges between DoD and the social science community. Minerva brings together universities, research institutions, and individual scholars and supports multidisciplinary and cross-institutional projects addressing specific topic areas determined by DoD.

Minerva projects are funded up to a five-year base period, with awards ranging from small, single investigator grants for 2-3 years to large multidisciplinary projects for $1-2 million per year for 5 years. The program is tri-service managed, with ARO managing 2-5 year projects dealing with causes and consequences of regime change, development of new models to pinpoint sources and effects of protest movements, relationships between natural disasters and sociopolitical instability, identification of demographic factors contributing to rise of global violent extremist organizations. ARO also provides scientific, technical, and managerial support to OSD in formulating the overall program.

The titles of ARO-managed FY15 new-start Minerva projects are listed below, followed by the name of the lead PI, the performing organization, and the award duration.

- *The Western Jihadism Data Collection,* PI: Professor Jyette Klausen, Brandeis University, FY15-FY16
- *International University Research Ventures: Implications for US Economic Competitiveness & National Security,* PI: Professor Mark Taylor, Georgia Institute of Technology, FY15-FY16
- *A Computational Model of Resources & Resiliency: Deploying the Elements of National Power for Strategic Influence,* PI: Professor William Rivera, Duke University, FY15-FY17
- *The Effects of Shocks on Overlapping and Functionally Interacting Social & Political Networks: A Multi-Method Approach*, PI: Professor Zeev Maoz, University of California - Davis, FY15-FY17
- *Minerva E-ID Assessment Framework (MEIA) Pilot Project*, PI: Professor Eric Burger, Georgetown University, FY15-FY16
- *Understanding China's Efforts to Becoming a Global Defense Science, Technology, & Innovation Leader*, PI: Professor Tai Ming Cheung, University of California – San Diego, FY15-FY17

VIII. SMALL BUSINESS INNOVATION RESEARCH (SBIR) AND SMALL BUSINESS TECHNOLOGY TRANSFER (STTR) PROGRAMS

Congress established SBIR and STTR programs in 1982 and 1992, respectively, to provide small businesses and research institutions with opportunities to participate in government-sponsored R&D. The DoD SBIR and STTR programs are overseen and administered by the Office of Small Business Programs within the Office of the Under Secretary of Defense for Acquisition, Technology and Logistics. The Army-wide SBIR Program is managed by RDECOM, while the Army-wide STTR Program is managed by ARO.

A. Purpose and Mission

The purpose of the SBIR and STTR programs is to (i) stimulate technological innovation, (ii) use small business to meet Federal R&D needs, (iii) foster and encourage participation by socially and economically disadvantaged small business concerns (SBCs), in technological innovation, and (iv) increase private sector commercialization of innovations derived from Federal R&D, thereby increasing competition, productivity, and economic growth. The STTR program has the additional requirement that small companies must partner with universities, federally funded research and development centers, or other non-profit research institutions to work collaboratively to develop and transition ideas from the laboratory to the marketplace.

B. Three-phase Process

The SBIR and STTR programs use a three-phase process, reflecting the high degree of technical risk involved in funding research, and developing and commercializing cutting edge technologies. The basic parameters of this three-phase process for both programs within the Army are shown in TABLE 1.

TABLE 1

Three-phase process of the SBIR and STTR programs. Phase I is an assessment of technical merit and feasibility, Phase II is a larger R&D effort often resulting in a deliverable prototype, and Phase III is a project derived from, extending, or logically concluding prior SBIR/STTR work, generally to develop a viable product or service for military or commercial markets.

	SBIR Contract Limits	STTR Contract Limits
Phase I	• 6 months, $100K max • 3-month option (at Government's discretion), $50K max, to fund interim Phase II efforts	• 6 months, $150K max • No options
Phase II	• 2 years, $1 million max	• 2 years, $1 million max
Phase III	• No time or size limit • No SBIR/STTR set-aside funds	• No time or size limit • No SBIR/STTR set-aside funds

1. Phase I. Phase I of the SBIR and STTR programs involves a feasibility study that determines the scientific, technical, and commercial merit and feasibility of a concept. Each SBIR and STTR solicitation contains topics seeking specific solutions to stated government needs. Phase I proposals must respond to a specific topic in the solicitation, and proposals are competitively judged on the basis of scientific, technical, and commercial merit. The Phase I evaluation and award process marks the entry point to the program and cannot be bypassed.

2. Phase II. Phase II represents a major research and development effort, culminating in a well-defined deliverable prototype (*i.e.*, a technology, product, or service). The Phase II selection process is also competitive. Phase I contractors can submit Phase II proposals during one of the respective program's submissions cycles, as there are no separate Phase II solicitations. Typically 50% of Phase II proposals are selected for award. SBIR Phase II awards may also be selected to receive additional funds as an invited Subsequent Phase II, Phase II Enhancement, or via the Commercialization Readiness Program (CRP).

3. Phase III. In Phase III, the small business or research institute is expected to obtain funding from the private sector and/or non-SBIR/STTR government sources to develop products, production, services, R&D, or any combination thereof into a viable product or service for sale in military or private sector markets. Commercialization is the ultimate goal of the SBIR and STTR programs.

C. ARO FY15 SBIR and STTR Topics

The following SBIR and OSD Defense Health Program SBIR topics were published in the FY15 SBIR solicitations. The lead topic author and corresponding Division are listed following each topic title.

- *Very High Dynamic Range RF Two Tone Measurement Instrument and Sensor*; Dr. James Harvey, Electronics
- *Wireless Networking Using Multiple Antenna Interference Alignment*; Dr. Robert Ulman, Network Sciences

- *High Operating Temperature Long Wave HgCdTe Focal Plane Arrays*; Dr. William Clark, Electronics
- *Enhanced Analysis for Pulsed Voltammetry Evaluation Tool / System For Improved Power Systems*; Dr. Robert Mantz, Chemical Sciences
- *Oxygen Separation from Air to Provide Supplemental Oxygen for Injured Soldiers*; Dr. Robert Mantz, Chemical Sciences

The following STTR topics were published in the FY15 STTR solicitations. The lead topic author and corresponding Division are listed following each topic title.

- *Intracavity Nonlinear Optical Generation of THz Radiation*; Dr. Michael Gerhold, Electronics
- *Stochastic Electromagnetic / Circuit Analysis*; Dr. James Harvey, Electronics
- *Terahertz Nano-Radio Platform with Integrated Antenna and Power Source*; Dr. Joe Qiu, Electronics
- *Novel Lightweight Thermoacoustic Materials and Processes for Noise Cancellation of Military Ground Combat Vehicles (GCV)*; Dr. Pani Varanasi, Materials Science
- *Compressive 3D Infrared Imaging*; Dr. Liyi Dai, Computing Sciences
- *EMS Monitor & Broadcast Training Capacity Enhancement*; Dr. Robert Ulman, Network Sciences
- *Compact Integrated Ion Trap Quantum Systems*; Dr. T.R. Govindan, Physics
- *Lithium Ion / Super Capacitor Hybrid System*; Dr. Robert Mantz, Chemical Sciences
- *Advanced Fibers for High Efficiency Capture and Release of Human Cellular Material for Forensic DNA Analysis*; Dr. Stephanie McElhinny, Life Sciences
- *Robust Training System for Autonomous Detectors*; Dr. Micheline Strand, Life Sciences

D. ARO FY15 SBIR and STTR Phase II Contract Awards

The following SBIR topics were selected for Phase II contracts in FY15. The lead topic author and corresponding Division are listed following each topic title.

- *Universal Software Assured Position, Navigation and Timing (USAPNT) Receiver*; Dr. Joe Qiu, Electronics
- *Novel Bioprocess for Spider Silk Fiber Production*; Dr. Stephanie McElhinny, Life Sciences

The following STTR topics were selected for Phase II contracts in FY15. The lead topic author and corresponding Division are listed following each topic title.

- *Ultra-Coherent Semiconductor Laser Technology*; Dr. Michael Gerhold, Electronics
- *Powerful Source of Collimated Coherent Infrared Radiation with Pulse Duration Fewer than Ten Cycles*; Dr. James Harvey, Electronics
- *High-Performance Magnesium Alloys and Composites by Efficient Vapor Phase Processing;* Dr. David Stepp, Materials Science
- *Low Power Monolayer MoS_2 Transistors for RF Applications* ; Dr. Pani Varanasi, Materials Science
- *Circadian Rhythm Monitoring and Regulation Device*; Dr. Virginia Pasour, Mathematical Sciences
- *Superconducting Parametric Amplifier*; Dr. TR Govindan, Physics
- *Pathogen Specific Antimicrobial Coatings For Fabrics*; Dr. Stephanie McElhinny, Life Sciences
- *Parallel Two-Electron Reduced Density Matrix Based Electronic Structure Software for Highly Correlated Molecules and Materials*; Dr. James Parker, Chemical Sciences
- *Innovative concept for detection and identification of biological toxins*; Dr. Dawanne Poree, Chemical Sciences

E. ARO FY15 SBIR Phase III Contract Awards

The following SBIR topics were awarded a Phase III contract in FY14 and FY15. The lead topic author and corresponding Division are listed following each topic title. Phase III revenues can be obtained from Government or private customers, but cannot be SBIR funds.

- *Fusing Uncertain and Heterogeneous Information - Making Sense of the Battlefield*; Dr. Purush Iyer, Network Sciences
- *Equipment Sets for Mitigating Advanced Threats*; Dr. Stephen Lee, Chemical Sciences
- *Advancement of Capabilities, Products, and Sensors in Chem/Bio Detection, Quantification, and Mitigation IDIQ*; Dr. Stephen Lee, Chemical Sciences

F. Contract Evaluation and Funding

The Army receives Phase I and Phase II proposals in response to SBIR, STTR, CBD-SBIR and OSD-SBIR/STTR topics that are published during specific solicitation periods throughout each fiscal year. Proposals are evaluated against published evaluation criteria and selected for contract award. Contract awards in the SBIR and STTR programs are made pending completion of successful negotiations with the small businesses and availability of funds. A summary of funds managed for ARO-managed SBIR and STTR contracts is provided at the end of this chapter.

IX. HISTORICALLY BLACK COLLEGES AND UNIVERSITIES AND MINORITY INSTITUTIONS (HBCU/MI) PROGRAMS

Programs for HBCU/MIs are a significant part of the ARO portfolio. Awards in FY15 totaled $13.5 million. These programs are discussed in the following subsections.

A. ARO (Core) HBCU/MI Program

ARO began its HBCU/MI program in 1980 with $0.5 million designed to encourage greater participation of HBCUs and MIs in basic research. The initiative has continued and in recent years has been funded at about $1.2 million annually. These funds are made available to the ARO scientific divisions as co-funding opportunities to support HBCU/MI research proposals submitted through the ARO Core Program BAA. There were 32 agreements with HBCU/MI institutions receiving over $12.4 million in funding through the ARO Core Program during FY15, including the 24 new starts. These figures represent total funding for HBCU/MIs through the core program, both awards relying on matching funds and those not utilizing matching funds.

The new-start HBCU/MI research grants are listed below, with the project title followed by the PI, performing organization, ARO PM, and corresponding scientific division.

- *Studies of Heat Transport and its Underlying Stochastic Dynamics in Smallest Thermal Engines: An Approach to Novel Form of Energy-Harvesting*, Professor Ilki Kim, North Carolina Agricultural and Technical State University; Dr. Robert Mantz, Chemical Sciences Division
- *A Study of GaAsSb Nanowire Photodetectors*, Professor Dr. Shanthi lyer, North Carolina Agricultural and Technical State University; Dr. William Clark, Electronics Division
- *High Order nonlinearly stable WENO schemes for the 3-D Navier-Stokes equation*, Professor Nail Yamaleev, North Carolina Agricultural and Technical State University; Dr. Joseph Myers, Mathematical Sciences Division
- *Instrument Development for a Long-Range, High-Resolution 3D Imaging Photon Counting LADAR*, Professor Renu Tripathi, Delaware State University; Dr James Parker, Chemical Sciences Division

- *Characterization of Nanowire Photodetectors*, Professor Shanthi Iyer, North Carolina Agricultural and Technical State University; Dr. William Clark, Electronics Division
- *Modeling, Fabrication and Characterization of Self- Aligned 2D and 3D Nanowire Arrays for Terahertz Operation*, Professor Arturo Ayon, University of Texas - San Antonio; Dr. Joe Qiu, Electronics Division
- *Organic-mediated Mineral Transport and Force Transduction in an Ultrahard Biological Composite: Biochemistry 8.1*, Professor David Kisailus, University of California- Riverside; Dr. Stephanie McElhinny, Life Sciences Division
- *TL/OSL Dating: Lattice Structure, Dating Accuracy, and Temporal Minima in Synthetic and Natural Models*, Professor David Sammeth, New Mexico Highlands University; Dr. David Stepp, Materials Science Division
- *A Local Analysis of the Fluid Dynamics and Flow Physics of Dynamic Stall on Helicopters*, Professor Andreas Gross; Dr. Matthew Munson, Mechanical Sciences Division
- *Understanding Knowledge Hoarding in Organizational Work Teams from a Transactive Memory and Social Network Perspective*, Professor Chunke Su, University of Texas - Arlington; Dr. Edward Palazzolo, Network Sciences Division
- *A Game Theoretic Approach To Self-Configuring, Non Cooperative Mobile Sensors For Monitoring Moving Targets*, Professor Sundararaj Iyengar, Florida International University; Dr. Cliff Wang, Computing Sciences Division
- *Mechanisms of Enhancing Impact Resistance of Layered Materials Using Thin Polymeric Interfaces*, Professor Luoyu Roy Xu, New Mexico State University; Dr. David Stepp, Materials Science
- *Dynamic Processes over Dynamic Social Networks*, Professor Francesco Bullo, University of California - Santa Barbara; Dr. Edward Palazzolo, Network Sciences Division
- *QUANTA: Quantitative Network-based Models of Adaptive Team Behavior*, Professor Ambuj Singh, University of California- Santa Barbara; Dr. Edward Palazzolo, Network Sciences Division
- *Building a Flexible Nework Infrastructure for Moving Target Defense*, Professor Srikanth Krishnamurthy, University of California – Riverside; Dr. Cliff Wang, Computing Sciences Division
- *In-situ integrating sphere apparatus for quantitative analysis of heterogeneous surfaces interacting with photons under controlled environments*, Professor Phillip Christopher, University of California - Riverside; Dr. Robert Mantz, Chemical Sciences Division
- *Alkaline Earth Quantum Gas Microscope for High-Resolution Imaging of Ultracold Strontium*, Professor David Weld, University of California - Santa Barbara; Dr. Paul Baker, Physics Division
- *Instrumentation for Exploring Surface Energy Balance using a combination of Satellite and Ground Based*, Professor Hamidreza Norouzi, CUNY-New York City College of Technology; Dr. Julia Barzyk, Materials Sciences Division
- *Acquisition of a Femtosecond Laser System for Materials Characterization and Education*, Professor Guillermo Bazan, University of California - Santa Barbara; Dr. J. Aura Gimm, Physical Sciences Directorate
- *A High Density Electrophysiological Data Analysis System for a Peripheral Nerve Interface Communicating with Individual Neurons in the Brain*, Professor Yoonsu Choi, University of Texas-Pan American; Dr. Frederick Gregory, Life Sciences Division
- *Dynamics and Control of Switching Dynamical Networks*, Professor Igor Belykh, Georgia State University; Dr. Randy Zachery, Information Sciences Directorate
- *Determination of Oxygen and Hydrogen Mass Transfer Coefficients in PEMFC GDE and Their Separation into Gas and Electrolyte Contributions*, Professor Tatyana Reshetenko, University of Hawaii; Dr. Robert Mantz, Chemical Sciences Division
- *Metal-Protein Interactions Coordinated by Beryllium Ion*, Professor Ronald Gary, University of Nevada - Las Vegas; Dr. Stephanie McElhinny, Life Sciences Division
- *Variations on Bayesian prediction and inference*, Professor Ryan Martin, University of Illinois - Chicago; Dr. Joseph Myers, Mathematical Sciences Division

The HBCU/MI institutions funded under the ARO Core program were also afforded the opportunity to submit add-on proposals to fund high school or undergraduate student research apprenticeships through HSAP/URAP. A total of seven HBCU/MIs were funded under HSAP/URAP in FY15, totaling approximately $57K, (50/50 mix of PM and Army Education Outreach Program funding). Additional information regarding HSAP/URAP can be found in Section XI: *Youth Science Activities*.

B. Partnership in Research Transition (PIRT) Program

The PIRT Program was established as the second phase of what was previously known as the Battlefield Capability Enhancement Centers of Excellence (BCE). The program's objective is to enhance the programs and capabilities of a select number of high-interest scientific and engineering disciplines through Army-relevant, topic-focused, near-transition-ready innovative research. Furthering ARL's policy of advocating and supporting research at HBCUs, and consistent with the stated mission of the White House Initiative on HBCUs, a secondary objective of PIRT is "to strengthen the capacity of HBCUs to provide excellence in education" and to conduct research critical to DoD national security functions. In FY15, $1.1 million was added to Cooperative Agreements supporting research and student internships at these PIRT Centers:

- *Center of Advanced Algorithms*
  Delaware State University, Dover, DE
  Co-Cooperative Agreement Manager (Co-CAM): Dr. James Harvey, Electronics
- *Bayesian Imaging and Advanced Signal Processing for Landmine and IED Detection Using GPR*
  Howard University, Washington, DC
  Co-CAM: Dr. James Harvey, Electronics
- *Extracting Social Meaning From Linguistic Structures in African Languages*
  Howard University, Washington, DC
  Co-CAM: Dr. Joseph Myers, Mathematical Sciences
- *Lower Atmospheric Research Using Lidar Remote Sensing*
  Hampton University, Hampton, VA
  Co-CAM: Dr. James Parker, Chemical Sciences
- *Nano to Continuum Multi-Scale Modeling Techniques and Analysis for Cementitious Materials Under Dynamic Loading*
  North Carolina A&T State University, Greensboro, NC
  Co-CAM: Dr. Joseph Myers, Mathematical Sciences

C. DoD Research and Educational Program (REP) for HBCU/MI

ARO has administered programs on behalf of ASD(R&E) since 1992. REP aims to enhance research capabilities of HBCUs and MIs and to strengthen their education programs in science, technology, engineering, and mathematics (STEM) disciplines that are relevant to the defense mission. The FY15 BAA solicited proposals from single investigators for basic research. Proposals were limited to three per eligible institution.

Under this program, qualifying institutions were able to submit proposals to compete for basic research grants. In 1Q FY15, BAA W911NF-15-R-0002 was issued for the FY15 DoD REP for HBCU/MI. One hundred twenty-one (121) proposals were determined to be eligible under the solicitation. " In FY15, 43 grants totaling $23.8M were made to 17 HBCUs, 25 MIs, and 1 TCU under the DoD REP solicitation.

D. Other HBCU/MI Activities

ARO continued to administer the John H. Hopps Scholars Program at Morehouse College (funded in FY08) continued to serve nine scholars during FY15. The Hopps Program ends in August 2016.

X. NATIONAL DEFENSE SCIENCE AND ENGINEERING GRADUATE (NDSEG) FELLOWSHIP PROGRAM

The NDSEG Fellowship Program is an OSD-funded program administered by AFOSR, designed to increase the number of US citizens trained in disciplines of science and engineering important to defense goals. ARO supports the NDSEG Fellowship Program along with ONR and AFOSR. NDSEG is a highly competitive fellowship awarded to U.S. citizens who have demonstrated a special aptitude for advanced training in science and engineering, and who intend to pursue a doctoral degree in one of fifteen scientific disciplines of interest to the military. NDSEG Fellowships last for three years, and Fellows are provided full tuition and fees at any accredited university of choice, a monthly stipend very competitive with other top-tier fellowships, and up to $1K/year in medical insurance.

With approximately $5 million available to the Army in FY15, ARO selected 64 NDSEG Fellows from thirteen categories relevant to Army fundamental research priorities. These awardees began their fellowships in the fall of 2013. Each of ARO's divisions reviewed the applications assigned to NDSEG topic categories within their particular areas of expertise, and selected fellows whose doctoral research topics most closely align with the Army's missions and research needs. The number of Fellows chosen from each discipline was based roughly on the percentage of applicants who submitted topics in that category. The number of fellows chosen from each scientific discipline for the FY15 NDSEG program is shown in TABLE 2.

TABLE 2

FY15 NDSEG fellows by discipline. The table displays the number of NDSEG Fellows chosen in FY15, according to topic categories relevant to the designated Army research priorities.

Scientific Discipline	NDSEG Fellows Selected in FY15
Aeronautical and Astronautical Engineering	4
Biosciences	9
Chemical Engineering	3
Chemistry	6
Civil Engineering	4
Cognitive, Neural, and Behavioral Sciences	6
Computer and Computational Sciences	5
Electrical Engineering	4
Geosciences	2
Materials Science and Engineering	4
Mathematics	3
Mechanical Engineering	5
Physics	5
TOTAL	**60**

XI. YOUTH SCIENCE ACTIVITIES

In FY14, several of the Army Educational Outreach Program (AEOP) programs previously managed by ARO were transferred to management by the STEM Outreach Office at RDECOM Headquarters. All the programs share one purpose: to increase the number of future adults with careers in science, technology, engineering, and mathematics. These programs accomplish this through a variety of mechanisms, including: providing a work/study laboratory experience, sponsoring hands-on science workshops during the summer, showcasing talented young high school scientists at symposia, and supporting student science fairs nationwide. Of these many programs, ARO continued to administer the High School and Undergraduate Research Apprenticeship Programs in FY15.

During the summer of FY15, 97 students served as interns and worked in university laboratories with mentors though the High School Apprenticeship Program (HSAP) and the Undergraduate Research Apprentice Program (URAP). This was a significant increase from the number of participants in FY14. These programs are described further in the following subsections.

A. Undergraduate Research Apprenticeship Program (URAP)

URAP funds the STEM apprenticeship of promising undergraduates to work in university-structured research environments under the direction of ARO-sponsored PIs serving as mentors. In FY15, URAP awards provided 48 students with research experiences at 36 different universities within 23 different states. Seven of the universities were HBCU/MIs and ARO invested approximately $174K in the FY15 URAP effort, a mix of ARO core funding and AEOP matching funds.

B. High School Apprenticeship Program (HSAP)

HSAP funds the STEM apprenticeship of promising high school juniors and seniors to work in university-structured research environments under the direction of ARO-sponsored PIs serving as mentors. In FY15, HSAP awards provided 48 students with research experiences at 28 different universities within 17 different states. Seven of the universities were HBCU/MIs. ARO invested approximately $149K in the FY15 HSAP effort, including ARO core funding and AEOP matching funds.

C. Youth Science Cooperative Outreach Agreement (YS-COA)

The YSCOA completed its fifth and final year of outreach efforts in FY15. It was awarded on 30 September 2010 (concluded 30 September 2015) to provide support and stimulation of STEM education and outreach in conjunction with DoD and the Army. YS-COA brought together government and a consortium of organizations working collaboratively to further STEM education and outreach efforts nationwide and consists of twelve major components, including the Junior Science and Humanities Symposium (JSHS), the Research and Engineering Apprenticeship Program (REAP), UNITE, Junior Solar Sprint (JSS), the Science and Engineering Apprentice Program (SEAP), College Qualified Leaders (CQL), Gains in the Education of Mathematical Sciences and Science (GEMS), and the ECybermission Internship Program (ECIP). As mentioned above, ARO's Co-Cooperative Agreement Manager (CAM) role migrated to RDECOM HQ in early FY14 as did programs for which ARO had a lead role (except HSAP and URAP).

Virginia Polytechnic Institute and State University led the consortium of non-profits and academic institutions to execute a collaborative STEM education and outreach program for the majority of FY15. Battelle was assigned as the new lead consortium in September, continuing the efforts of focusing on AEOP core objectives:

- STEM Literate Citizenry: Broaden, deepen, and diversify the pool of STEM talent in support of our Defense Industry Base (DIB)
- STEM "Savvy" Educators: Support and empower educators with unique Army Research and Technology Resources

- Develop and implement a cohesive, coordinated, and sustainable STEM education outreach infrastructure across the Army

The major accomplishments in FY15 included year-end program reviews with Individual Program Administrators (IPAs), Cooperative Agreement Consortium Meeting and Army Cooperative Agreement and subject matter experts, as well as the release of the AEOP Abstract Book, and AEOP Marketing Products.

D. Thurgood Marshall College Fund Pilot Initiative

The Vivian Burey Marshall Academy (VBMA), named in honor of Justice Thurgood Marshall's first wife, is a two-tiered, pilot initiative grant awarded to the Thurgood Marshall College Fund in late FY15. This is a four-year research grant award up to $5.7 million funded by ASA (ALT) through ARL's Broad Agency Announcement and consistent with the goals of the AEOP. The pilot initiative will develop in young students, grades 6-10, STEM literacy and the basic underlying skills necessary for STEM management.

The pilot effort will be evaluated throughout the 4-year implementation to assess impact and feasibility of program adoption. ASA (ALT) has requested Army S&T organizations support VBMA sites for the initial year: RDECOM with Baltimore, MD, and ERDC with Vicksburg, MS.

E. Local Outreach

The Youth Sciences division of ARO participated in the following local outreach efforts in FY15.

- North Carolina Science and Engineering Fair: ARO PMs volunteered to judge posters for a special category that presents awards to high school juniors and seniors based upon the overall quality and Army relevance of their projects.
- JSHS National Symposium: scientists from ARO and sponsored PIs attended and judged student posters as well as oral presentations of students that have previously won regional competitions. Winners are awarded various scholarships ranging from $4,000 to $12,000; ARO technical staff also participated to assist with event logistics.
- Site visits to local universities that host HSAP/URAP participants: the HSAP/URAP Program Coordinator visited host sites within North Carolina to measure program efficacy. An ARO PM accompanied the Program Coordinator on one visit.

XII. SCIENTIFIC SERVICES PROGRAM (SSP)

ARO established the SSP in 1957. This program provides a rapid means for the Army, DoD, OSD, and other federal government agencies to acquire the scientific and technical analysis services of scientists, engineers, and analysts from small and large businesses, colleges and universities, academicians working outside their institutions, and self-employed persons not affiliated with a business or university. Annual assistance is provided through the procurement of short-term, engineering and scientific technical services in response to user-agency requests and funding. Through the SSP, these individuals provide government sponsors with scientific and technical results and solutions to problems related to R&D by conducting well-defined studies, analyses, evaluations, interpretations, and assessments in any S&T area of interest to the government.

SSP services are administered and managed for ARO through the Battelle Eastern Science and Technology (BEST) Center located in Aberdeen, Maryland on behalf of Battelle Memorial Institute (BMI), headquartered in Columbus, Ohio. Battelle's responsibilities include the selection of qualified individuals, universities, businesses, and/or faculty to perform all tasks requested by ARO, and for the financial, contractual, security, administration, and technical performance of all work conducted under the program.

SSP awards tasks in a wide variety of technical areas, including mechanical engineering, computer sciences, life sciences, chemistry, material sciences, and military personnel recruitment/retention. In FY15, 56 new SSP tasks were awarded in addition to 101 modifications of the scope and/or funding of ongoing tasks on two SSP contracts. A summary of the agencies served under this program and the corresponding number of FY15 new SSP tasks is provided in TABLE 3.

TABLE 3

FY15 SSP tasks and sponsoring agencies. In FY15, 56 new SSP tasks were awarded in addition to 101 modifications of the scope and/or funding of ongoing tasks on two SSP contracts.

Sponsoring Organization	SSP Tasks
Army Research, Development and Engineering Command (RDECOM)	
Army Research Laboratory (ARL)	9
Edgewood Chemical, Biological Center (ECBC)	8
Research, Development, and Engineering Centers (RDECs)	
Army Missile RDEC (AMRDEC)	4
Armaments RDEC (ARDEC)	1
Natick Soldier RDEC (NSRDEC)	7
Communications-Electronics RDEC (CERDEC)	1
Tank-Automotive RDEC (TARDEC)	1
TOTAL: RDECOM	**31**
Other U.S. Army	
US Military Academy (USMA)	4
Headquarters Department of Army (HQ DA)	5
Program Executive Office Combat Support & Combat Service Support	1
US Army Corps of Engineers (USACE)	4
US Army Training & Doctrine Command (TRADOC)	2
US Army Aeromedical Research Laboratory (AARL)	1
TOTAL: Other U.S. Army	**17**
Other DoD	
US Air Force	2
US Navy	3
DoD (Other)	2
Department of Homeland Security	1
TOTAL: Other DoD	**8**
TOTAL FY15 SSP Tasks	**56**

XIII. SUMMARY OF PROGRAM FUNDING AND ACTIONS

A. FY15 Research Proposal Actions

ARO PMs receive white papers throughout the year and discuss these topic ideas with the potential investigator to identify any ways the proposed research could better align with program vision and Army needs. PMs then encourage a subset of white papers to be submitted as full proposals; however, any eligible investigator can submit a full proposal, regardless of PM recommendations. On average, one-fifth of the white papers received by ARO PMs are ultimately submitted as formal, full proposals.

The actions for FY15 extramural basic research full proposal submissions, sorted by ARO Division, are summarized in TABLE 4.

TABLE 4

FY15 ARO Research Proposal Actions. The status of research proposals submitted to ARO (i.e., received) within FY15 (*i.e.*, 1 Oct 2014 through 30 Sep 2015) is listed for each scientific division, based on proposal actions reported through 5 May 2016. The table reports actions for extramural proposals in the 6.1 basic research categories: SI, STIR, YIP, HBCU/MI Core, MRI, MURI, and DURIP.

	Received	Accepted	Declined	Pending	Withdrawn
Chemical Sciences	149	65	54	30	0
Computing Sciences	76	51	11	14	0
Electronics	117	58	43	16	0
Life Sciences	150	63	66	21	0
Materials Science	107	39	55	12	1
Mathematical Sciences	51	35	3	13	0
Mechanical Sciences	119	53	59	6	1
Network Sciences	57	36	16	4	1
Physics	108	46	42	20	0
TOTAL	**934**	**446**	**349**	**136**	**3**

B. Summary of ARO Core Program Budget

The ARO FY15 Core (BH57) Research Program budget is shown in TABLE 5, below.

TABLE 5

ARO Core (BH57) Program funding. The ARO Core Program FY15 Budget is listed according to each scientific discipline (Division) or special program; data sources: ARO Director's Budget (for scientific disciplines) and Status of Funds Report 31 Jan 2016 (for special programs).

ARO Core (BH57) Program Type	Division or Program Title	FY15 Allotment
Scientific Disciplines	Chemical Sciences[1]	$8,231,846
	Computing Sciences	$5,094,810
	Electronics	$6,217,641
	Life Sciences	$7,355,867
	Materials Science[1]	$7,027,398
	Mathematical Sciences	$5,850,735
	Mechanical Sciences	$6,795,482
	Network Sciences	$5,924,755
	Physics	$7,245,912
	SUBTOTAL: Core Program Funding by Scientific Discipline	**$59,744,446**
Special Programs	Senior Scientist Research Programs	$905,084
	National Research Council (NRC) Associates Program	$361,401
	HBCU/MI Program[2,3]	$1,012,682
	HSAP/URAP	$172,023
	In-House Operations	$16,296,895
	SUBTOTAL: Core Program Funding to Special Programs	**$18,748,085**
TOTAL	**ARO Core (BH57) Program**	**$78,492,531**

[1] Includes funding for some projects that began under the former Environmental Sciences Division, now temporarily managed within these other Divisions.

[2] HBCU/MI Core Program funds are allocated at the Directorate level, and are matched with Division funds, resulting in total FY15 HBCU/MI Core Program funding of $2.0M.

[3] Does not include the additional funds provided from OSD for the HBCU/MI Program (see TABLE 8).

C. Summary of Other Programs Managed or Co-managed by ARO

The FY15 allotments and funding sources for other ARO managed or co-managed programs (*i.e*, not part of the ARO Core Program), are shown in TABLES 6-8.

TABLE 6

FY15 allotments for other Army-funded programs. These programs, combined with the ARO Core (BH57) Program elements shown in TABLE 5, represent all of the Army-funded programs managed through ARO. Data source: 31 Jan 2016 Status of Funds Report and 30 Sep 2015 Status of Funds Report (for FY14 funds received in or reallocated for FY15).

Other Army-funded Program	FY15 Allotment
Multidisciplinary University Research Initiative	$44,408,695
Presidential Early Career Award for Scientists and Engineers	$2,994,924
Defense University Research Instrumentation Program	$13,997,187
University Research Initiative Support	$3,299,194
MINERVA Program (Project V72)[1]	$2,383,180
Army Center of Excellence (Project H59)	$394,000
HBCU/MI – PIRT Centers (Project H04)	$2,998,227
Institute for Collaborative Biotechnologies (ICB; Project H05)	$7,692,000
Institute for Soldier Nanotechnologies (ISN; Project J12)	$6,454,000
Institute for Creative Technologies (ICT; Project J08)	$7,210,000
Board of Army Science and Technology (BAST; Project C18)	$961,000
Small Business Innovation Research (SBIR; Project M40)[1,2]	$5,383,532
Small Business Technology Transfer (STTR; Project 861)[1,3]	$12,676,200
SBIR/STTR Services / Contract Support (Project 720)	$814,000
Basic Research Initiatives – Congressional (T14)	$10,250,000
University Research Initiatives – Congressional (D58)	$12,000,000
Communications and Electronics RDEC (CERDEC)	$2,747,364
TOTAL: Other Army-funded Programs	**$136,663,503**

[1] Does not include additional funds provided by OSD (see TABLE 8).
[2] Includes $4,409,047 of FY14 funds received in or reallocated for FY15
[3] Includes $2,163,894 of FY14 funds received in or reallocated for FY15

TABLE 7

FY15 allotment for externally-funded programs. FY15 funds received from sources other than Army or OSD are indicated below. The Other Agencies category totals the funds from a range of sources, including the Joint IED Defeat Organization (JIEDDO), the Joint Project Manager, Nuclear, Biological, and Chemical (JPMNBC), and other government agencies. Data source: 31 Jan 2016 Status of Funds Report and 30 Sep 2015 Status of Funds Report (for FY14 funds received in or reallocated for FY15).

External Program	FY15 Allotment
Scientific Services Program (SSP)[1]	$17,912,608
Defense Advanced Research Projects Agency (DARPA)[2]	$132,961,186
Air Force Research Laboratory (AFRL)	$5,964,474
Office of Naval Research (ONR)[3]	$5,930,112
Other Agencies (*e.g.*, JIEDDO and JPMNBC)	$47,418,726
Other DoD	$8,256,764
TOTAL: External Programs	**$218,443,870**

[1] Includes $1,486,049 of FY14 funds received in or reallocated for FY15
[2] Includes $9,237,634 of FY14 funds received in or reallocated for FY15
[3] Includes $1,173,404 of FY14 funds received in or reallocated for FY15

TABLE 8

OSD direct-funded programs. These funds were allocated directly from OSD to the indicated program. Data source: 31 Jan 2016 Status of Funds Report.

OSD Direct-funded Programs	FY15 Allotment
SBIR/STTR (Project 8Z5)[1,2]	$1,526,959
Chemical and Biological Defense Programs (Project BP0)[2]	$2,135,465
HBCU/MI and Research and Educational Program (REP)[3]	$27,116,670
Minerva[4]	$1,855,229
TOTAL: OSD Direct Funding	**$32,634,323**

[1] Does not include additional Army funds provided for SBIR/STTR (see TABLE 6).
[2] FY14 funds received in or reallocated for FY15
[3] This amount does not include the additional Army Core Program funds provided for the HBCU/MI Program (see TABLE 5).
[4] Includes $844,935 of FY14 funds received in or reallocated for FY15

D. Grand Total FY15 Allotment for ARO Managed or Co-managed Programs

TABLE 9

Summary of FY15 allotment for all ARO managed or co-managed programs. This table lists the subtotals from TABLES 6-9 and the grand total FY15 allotment for all ARO managed or co-managed programs, including any FY14 funds received in or allocated for FY15.

Program Category	FY15 Allotment
Core (BH57) Programs	$78,492,531
Other Army-funded Programs	$136,663,503
External Program Funds	$218,443,870
OSD Direct-funded Programs	$32,634,323
GRAND TOTAL: (all sources)	**$466,234,227**

CHAPTER 3: CHEMICAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2015* is to provide information on the programs and basic research supported by ARO in FY15, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Chemical Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY15.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Chemical Sciences Division supports research to identify and control the fundamental properties, principles, and processes governing molecules and their interactions in materials and chemical systems that will ultimately enable critical new Army capabilities. More specifically, the Division promotes basic research to uncover the relationships between molecular architecture and material properties, to understand the fundamental processes of electrochemical reactions, to develop methods for accurately predicting the pathways, intermediates, and energy transfer of reactions, and to discover and characterize the many chemical processes that occur at surfaces and interfaces. The results of these efforts will stimulate future studies and help keep the U.S. at the forefront of chemical sciences research. In addition, these efforts are expected to lead to new approaches for synthesizing and analyzing molecules and materials that will open the door to future studies that are not feasible with current knowledge.

2. Potential Applications. Research managed by the Chemical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, results from the Chemical Sciences Program may lead to materials with new or enhanced properties to protect the Soldier from ballistic, chemical, and biological threats. The development of new computational methods may allow the structure and properties of notional (*i.e.*, theoretical) molecules to be calculated before they are created, providing a significant cost savings to the Army. In addition, chemical sciences research may ultimately improve Soldier mobility and effectiveness through the development of light-weight and small power sources, renewable fuel sources, and new energetic materials with improved methods for ignition, detonation, and control.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Chemical Sciences Division coordinates and leverages research within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), and the Air Force Office of Scientific Research (AFOSR). In addition, the Division coordinates with other ARO Divisions to co-fund research, identify multidisciplinary research topics, and to evaluate the merit of research concepts. For example, interactions with the ARO Life Sciences Division include developing research programs to investigate materials for use in chemical and biological defense and to understand how biological systems can interface with or expand the capabilities of abiotic systems. The Chemical Sciences Division also coordinates its research portfolio with the Materials Science Division to pursue the design and characterization of novel materials through new synthesis and processing methods, the evaluation of bulk mechanical properties, and molecular-level studies of materials and material properties. Research in chemical sciences also complements research in the Physics and Electronics Divisions to investigate the dynamics of chemical reactions and how chemical structure influences electrical, magnetic, and optical properties. The creation of new computational methods and models to better understand molecular structures and chemical reactions is also an area of shared interest between the Chemical Sciences and Mathematical Sciences Divisions. Research in the Chemical Sciences Division is also coordinated with research in the

Atmospheric Sciences Program (of the former Environmental Sciences Division; refer to CHAPTER 1, Section V), in which new methods and reactions are being explored for detecting, identifying, and neutralizing toxic materials. These interactions promote a synergy among ARO Divisions, providing a more effective mechanism for meeting the long-term needs of the Army.

B. Program Areas

The Chemical Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the identification, evaluation and monitoring of research projects. In FY15, the Division managed research within these five Program Areas: (i) Polymer Chemistry, (ii) Molecular Structure and Dynamics, (iii) Electrochemistry, and (iv) Reactive Chemical Systems. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Polymer Chemistry. The goal of this Program is to understand the molecular-level link between polymer microstructure, architecture, functionality, and the ensuing macroscopic properties. Research in this Program may ultimately enable the design and synthesis of functional polymeric materials that give the Soldier new and improved protective and sensing capabilities as well as capabilities not yet imagined. This Program is divided into two research thrusts: (i) Precision Polymeric Materials and (ii) Complex Polymer Systems. The Precision Polymeric Materials thrust supports research aimed at developing new approaches for synthesizing polymers with precisely-defined molecular weight, microstructure (monomer sequence and tacticity), architecture, and functional group location; exploring how changes in molecular structure and composition impact macroscopic properties; and on developing polymers that exhibit programmed molecular responses to external stimuli. Of particular interest is research related to sequence-defined polymers, self-immolative polymers, and polymer mechanochemistry. The Complex Polymer Systems thrust focuses on controlling polymer assembly to enable complex structures with diverse functions and new properties. Of interest to this thrust are research efforts that explore how molecular structure influences polymer assembly into more complex, hierarchical structures as well as influence interactions with other materials (*i.e.* inorganic or biological materials) to render functional hybrid assemblies. Research efforts that explore assembly/incorporation of multiple responsive groups into a single polymeric materials system to engender complex responsive behavior are also of interest.

The research supported by this Program Area may lead to long-term applications for the Army such as light-weight, flexible body armor, materials for clothing that are breathable but also provide protection from toxins, fuel cell membranes to harness renewable energy, and damage-sensing and self-healing materials for vehicles, aircraft, and other DoD materiel. In addition, the efforts in this program may ultimately lead to new, dynamic materials such as photohealable polymers that can be used as a repairable coating and mechanically- or thermally-responsive polymers and composites that can convert external forces to targeted internal chemical reactions (*i.e.*, to convert external force to internal self-sensing and self-repair).

2. Molecular Structure and Dynamics. The primary goal of this Program Area is to understand state-selected dynamics of chemical reactions of molecules in gas and condensed phases across a wide variety of conditions (temperatures and pressures), and to develop theories that are capable of accurately describing and predicting these phenomena. In the long term, these studies may serve as the basis for the design of future propellants, explosives, and sensors. This Program Area is divided into two research Thrusts: (i) Molecular Dynamics and (ii) Quantitative Theoretical Methods. The Molecular Dynamics Thrust broadly supports research on the study of energy transfer mechanisms in molecular systems (reactive and non-reactive). The Quantitative Theoretical Methods Thrust supports research to develop and validate theories for quantitatively describing and predicting the properties of chemical reactions and molecular phenomena.

The research supported by this Program Area will likely enable many future applications for the Army and general public. These applications include more efficient and clean combustion technology, the development of new tools to study condensed phases of matter, the capability to accurately predict the properties of large, complex chemical systems, and the development of novel molecules for use in energy storage applications.

3. Electrochemistry. The goal of this Program Area is to understand the underlying science that controls reactant activation and electron transfer. These studies may provide the foundation for developing advanced power generation and storage technology. This Program Area is divided into two research Thrusts: (i) Reduction-oxidation (Redox) Chemistry & Electrocatalysis, and (ii) Transport of Electroactive Species. The Redox Chemistry and Electrocatalysis thrust supports research efforts to discover new spectroscopic and electrochemical techniques for probing surfaces and selected species on those surfaces, while the Transport of Electroactive Species thrust identifies and supports research to uncover the mechanisms of transport through polymers and electrolytes, to design tailorable electrolytes based on new polymers and ionic liquids, and also explores new methodologies and computational approaches to study the selective transport of species in charged environments.

Research in this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications include the discovery and use of new mechanisms for the storage and release of ions that are potentially useful in future power sources, including new battery or bio-fuel concepts. In addition, studies of electroactive species may enable the development of multifunctional materials that simultaneously have ionic conductivity, mechanical strength, and suitable electronic conductivity over a considerable temperature range, while exposed to aggressive chemical environments.

4. Reactive Chemical Systems. The goals of this Program Area are to obtain a molecular level understanding of interfacial activity and of dynamic nanostructured and self-assembled chemical systems. High-risk basic research in this program is expected to lead to the design and synthesis of new chemical systems that will provide unprecedented hazardous materials management capabilities and soldier survivability. This Program Area is divided into two research Thrusts: (i) Interfacial Activity and (ii) Synthetic Molecular Systems. Within these Thrusts, high-risk, high-payoff research efforts are identified and supported to pursue the program's long-term goals. The Interfacial Activity Thrust supports research on understanding the kinetics and mechanisms of reactions occurring at surfaces and interfaces and the development of new methods to achieve precise control over the structure and function of chemical and biological molecules on surfaces. Specific areas of interest include adsorption, desorption, and the catalytic processes occurring at surfaces and interfaces and the interface between nanostructures and biomolecules to generate advanced materials. Research in the Synthetic Molecular Systems Thrust is exploring novel methods for incorporation of multi-functionality, stimuli-responsive, and dynamic behavior into chemical systems. Specific areas of interest include the stabilization of nanostructured and self-assembled systems, incorporation of enhanced catalytic activity into chemical systems, and the design and synthesis of chemical systems that sense and respond to specific external stimuli.

This Program Area supports research that will likely lead to many long-term applications for the Army and the private sector. Potential long-term applications include novel chemical sensing capabilities, selective membranes, multi-functional surfaces for self-repair and self-healing, and new approaches to hazardous waste management. Research in these areas may also lead to multi-functional and stimuli-responsive systems for "smart" materials that can sense and autonomously respond in unprecedented ways for soldier protection.

C. Research Investment

The total funds managed by the ARO Chemical Sciences Division for FY15 were $39.1 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY15 ARO Core (BH57) program funding allotment for this Division was $8.9 million, which included a non-recurring annual increase of $1.0 million. The. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $9.5 million to projects managed by the Division. The Division also managed $4.3 million of Defense Advanced Research Projects Agency (DARPA) programs, and $2.3 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $2.2 million for contracts. The Institute for Soldier Nanotechnologies received $7.9 million. Finally, $4.2 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.2 million of ARO Core (BH57) funds, in addition to funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY15 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY15 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY15, the Division awarded 21 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Christopher Alabi, Cornell University; *Sequence Defined Polymers And Their Structural Evaluation*
- Professor Charles Angell, Arizona State University; *Fundamental Studies on the Dynamics and Energetics of Protic Ionic Liquids*
- Professor Ivan Aprahamian, Dartmouth College; *Dynamic Control of Self-Organized Assemblies using Near Infrared and Visible Light Activated Azo-BF2 Switches*
- Professor Andrew Boydston, University of Washington; *Exploring Mechanaphore and Polymer Design Rules for Mechanochemical Transduction*
- Professor Jeffery Byers, Boston College; *Redox-Switchable Polymerization for the Synthesis of High Performance Polymers*
- Professor Seth Cohen, University of California - San Diego; *The Chemistry of Metal Organic Frameworks Captured by Liquid and Gas Phase in Situ TEM*
- Professor Stephen L. Craig, Duke University; *Stress-strengthening Synthetic Polymers by Covalent Mechanochemistry*
- Professor Hai-Lung Dai, Temple University; *Enhancing Interfacial Charge Carrier Injection in Semiconductor Nanostructures*
- Professor Elena Jakubikova, North Carolina State University; *Toward the Computational Design of Iron-Based Chromophores*
- Professor Joel Kaar, University of Colorado - Boulder; *Single Molecule Resolution of Immobilized Enzyme Function*
- Professor James McCusker, Michigan State University; *Studies of Ultrafast Interfacial Electron Transfer Dynamics in Semiconductor-Chromophore Assemblies based on Earth-abundant Materials*

- Professor Josef Michl, University of Colorado - Boulder; *Porphene: A Regular Heterocyclic Analog of Graphene*
- Professor Chad Mirkin, Northwestern University Evanston Campus; *Infinite Coordination Polymer Particles from Polymeric Coordinating Precursors*
- Professor Mark Mirotznik, University of Delaware; *Design and Fabrication of Nano-plasmonic Surfaces*
- Professor Stuart Rowan, Case Western Reserve University; *One-Component Composites based on Nanorods: From fundamental studies to multifunctional materials*
- Professor Jonathan Rudick, SUNY - Stony Brook; *Synthesis Of Novel Dendritic Materials With Precise Control In Positioning Of Multifunctional Functional Groups*
- Professor Shouheng Sun, Brown University; *New Composite Catalysts Based on Nitrogen-Doped Graphene and Nanoparticles for Advanced Electrocatalysis*
- Professor YuYe Tong, Georgetown University; *Parsing the New Chemistry of Methanol and Formic Acid Oxidation Reactions on Pt-based Electrocatalysts by in situ Spectroelectrochemistry and Density Functional Theory Calculations*
- Professor Chunsheng Wang, University of Maryland - College Park; *Electrode/Electrolyte Interface of All Garnet Solid State Li-ion Batteries*
- Professor Sharon Weiss, Vanderbilt University; *Molecule-Surface Dynamics in Functionalized Mesoporous Silicon*
- Professor Richard Zare, Stanford University; *Reaction Dynamics Using a Coherent M-state Superposition Within a Single (v, J) Rovibrational Energy Eigenstate*

2. Short Term Innovative Research (STIR) Program. In FY15, the Division awarded 12 new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor S. Allen, University of California - Santa Barbara; *Dielectric Sensing via Impedance Spectroscopy and Plasmonic Resonance*
- Professor Guillermo Bazan, University of California - Santa Barbara; *Electrode-Specific Molecular Wires for Bioelectrochemical Systems*
- Professor Phillip Christopher, University of California - Riverside; *Digital Control of Reaction Cascades via Plasmon Activated Biocatalysis*
- Professor Seth Cohen, University of California - San Diego; *Metal-Organic Framework-based Mixed-Matrix Membranes for Hazardous Chemical Capture*
- Professor Laura Fabris, Rutgers, The State University of New Jersey - New Brunswick; *Use of Gold Nanorods for Fine Tunable Strain Strengthening of Synthetic Poly-isoprene*
- Professor Nathan Gianneschi, University of California - San Diego; *Growth on Treated Surfaces and Degradation Under Various Conditions of Metal Organic Frameworks Captured by In Situ Liquid TEM*
- Professor Thomas Harris, Northwestern University Evanston Campus; *Heme-Containing MOFs*
- Professor Ive Hermans, University of Wisconsin - Madison; *Insights in Catalytic Transformations at the Solid-liquid Interface*
- Professor Weiguo Hu, University of Massachusetts - Amherst; *Molecular Dynamics and Morphology of High-Performance Elastomers and Fibers by Solid-State NMR*
- Professor Stephen Paddison, University of Tennessee at Knoxville; *Quantitative Determination of Partial Structure Factors for Polymerized Ionic Liquids with Molecular Dynamics Simulations*
- Professor Edmund Palermo, Rensselaer Polytechnic Institute; *Sequence-Controlled Polymerization on Facially Amphiphilic Templates at Interfaces*
- Professor Orlin Velev, North Carolina State University; *Novel Magnetically Responsive and Self-repairing Particle-lipid-water Gels*

3. Young Investigator Program (YIP). In FY15, the Division awarded one new YIP project to drive fundamental research in areas relevant to the current and future Army. The following PI and corresponding organization were awarded the new-start YIP project.

- Professor Chao Wang, Johns Hopkins University; *Novel Bifunctional Electrocatalysts Based on Heterodimer Nanoparticles*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY15 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Polymer Electrolyte Fuel Cells Symposium at the 226th Meeting of the Electrochemical Society*; Cancun, Mexico; 5-10 October 2014
- *Nineteenth International Symposium on Molten Salts and Ionic Liquids at the 226th Meeting of the Electrochemical Society*; Cancun, Mexico; 5-10 October 2014
- *Symposium Z: Materials Challenges for Energy Storage Across Multiple Scales*; *Fall 2014 MRS Meeting*; Boston, MA; 30 November - 5 December 2014
- *2015 Center for Electrochemistry Annual Workshop on Electrochemistry*; University of Texas at Austin; 7-8 February 2015
- *Design Principles of Functional Macromolecular Materials symposium at the 249th ACS National Meeting*; Denver CO; 22-26 March 2015
- *Fifth International Conference on Attosecond Physics*; Manior Saint-Sauver, Saint-Sauver, Canada; 6-10 June 2015
- *2015 Gordon Research Seminar on Polymers*; South Hadley, MA; 13-14 June 2015
- *2015 Gordon Research Conference on Liquid Crystals*; Biddeford, ME; 20-26 June 2015
- *Conference on Dynamcis of Molecular Collisions*; Asilomar, California; 12-17 July 2015
- *20th International Conference on Solid State Ionics*; Keystone, CO; 15-19 July 2015
- *Gordon Research Conference on Quantum Control of Light and Matter*; Mount Holyoke College, South Hadley, Massachussetts; 2-7 August 2015
- *33rd International Symposium on Free Radicals*; Squaw Valley, California; 2-7 August 2015
- *Operando Spectroscopic Approach to Quantifying Structure-Activity Relationships of Real Catalysts Under Ambient Conditions symposium at the 250th ACS National Meeting*; Boston, MA; 16-20 August 2015
- *Ionic Liquids in Polymer Design: From Energy to Health symposium at the 250th ACS National Meeting*; Boston, MA; 16-20 August 2015

5. Special Programs. In FY15, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded 11 new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These projects constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Molecular Design of Novel Fibers using Carbon Nonotubes. This MURI began in FY09 and was awarded to a team led by Professor Horacio Espinosa at Northwestern University. The focus of this MURI is to understand the molecular properties required for preparing strong fibers using polymers and double-walled carbon nanotubes (DWCNT).

The chief objectives of this research are to (i) develop a model system for predicting the molecular properties necessary for preparing new, high-strength fibers, and (ii) to prepare novel fibers composed of double-walled carbon nanotubes and polymers. The team will use multiscale computer simulations to bridge atomistic (*i.e.*, electronic structure methods and reactive force fields), coarse-grain, and continuum scales to explore and understand DWCNT-polymer interactions, crosslinking effects (bond-breaking mechanisms), and the impact of architecture on fiber strength, elasticity, and toughness. The investigators will use the results to predict fiber precursor properties necessary for optimum strength. The team will use predictive models to develop chemical vapor deposition techniques for producing highly-aligned DWCNT mats with optimized density and surface chemistry. The mats will serve as precursors for fiber formation. These materials will be characterized using *in situ* and *ex situ* microscopy (*i.e.*, assayed during and after reaction completion). The fundamental scientific knowledge uncovered through this research may lead to new approaches for designing and preparing high-strength, flexible fibers that are directly relevant to lighter-weight and flexible personnel armor.

2. Ion Transport in Complex Organic Materials. This MURI began in FY10 and was awarded to a team led by Professor Andrew Herring at the Colorado School of Mines. This MURI team is investigating the interplay of chemical processes and membrane morphology in anion exchange.

Ion transport in complex organic materials is essential to many important energy conversion approaches. Unfortunately, ion transport is poorly understood in terms of its relationship to water content, morphology, and chemistry. While a great deal of research has focused on proton exchange membranes, little work has been performed with anion exchange membranes. This MURI team is studying the fundamentals of ion transport by developing new polymer architectures (*e.g.*, polymer membranes) using standard and novel cations. These new polymer architectures and aqueous solutions containing representative cations will serve as a model system for studies of anion transport and its relationship to polymer morphology. In the longer term, the design and synthesis of robust, thin alkali-exchange membranes, combined with an improved understanding of ion exchange gained through the characterization of these membranes, could enable the development of new classes of fuel cells. If the MURI team can characterize the fundamental processes of ion exchange across these polymer membranes, future fuel cells using similar membranes could harness alkali exchange, resulting in inexpensive, durable, and flexible-source power for the Army and commercial use.

3. Peptide and Protein Interactions with Abiotic Surfaces. This MURI began in FY11 and was awarded to a team led by Professor Zhan Chen at the University of Michigan, Ann Arbor. This MURI is exploring the processes that occur at biological/abiological interfaces. This research is co-managed by the Chemical Sciences and Life Sciences Divisions.

The objective of this research is to develop a systematic understanding of biological/abiological interfaces and how to design systems for predicted biological structure and function. The MURI team is using a combination of modeling and experimental techniques to understand the interactions of peptides and proteins covalently immobilized on abiotic surfaces. Specifically, the team will be investigating two peptides and one enzyme, with a variety of surfaces, such as self-assembled monolayers, chemically functionalized liquid crystalline films, and chemical vapor deposited polymers. The immobilized biological species will be characterized to determine not only structure but also activity. The investigators will utilize systematic modifications of the surface to probe the effect of chemical composition, morphology, and hydrophobicity on biological structure and function. The role of water will also be probed to determine how hydration affects not only immobilization, but also structure and function. Results from this research may ultimately enable the incorporation of nanostructured abiotic/biotic materials in applications such as sensing, catalysis, coatings, drug delivery, prosthetics, and biofilms.

4. High-Resolution Quantum Control of Chemical Reactions. This MURI began in FY12 and was awarded to a team led by Professor David DeMille at Yale University. This MURI is exploring the principles of ultracold molecular reaction, where chemical reactions take place in the sub-millikelvin temperature regime. This research is co-managed by the Chemical Sciences and Physics Divisions.

The study of ultracold molecular reactions, where chemical reactions take place in the sub-millikelvin temperature regime, has emerged as a new field in physics and chemistry. Nanokelvin chemical reactions are radically different than those that occur at “normal” temperatures. Chemical reactions in the ultracold regime can occur across relatively long intermolecular distances, and no longer follow the expected (Boltzmann) energy distribution. The reactions become heavily dependent on nuclear spin orientation, interaction strength, and correlations. These features make them a robust test bed for long-range interacting many-body systems, controlled reactions, and precision measurements.

The objectives of this MURI are to develop a fundamental understanding of the nature of molecular reactions in the nanokelvin temperature regime and to extend the cooling technique previously demonstrated by Professor DeMille[1] (through a previous ARO award) to other molecular candidates. The researchers will focus will be on the implementation of novel and efficient laser cooling techniques of diatomic molecules, and to understand the role of quantum effects, including the role of confined geometries, on molecules that possess vanishingly-small amounts of thermal energy. This research could ultimately lead to new devices or methods that explicitly use quantum effects in chemistry, such as the precision synthesis of mesoscopic samples of novel molecular compounds, new avenues for detection of trace molecules, and a new understanding of combustion and atmospheric chemical reactions.

5. Coherent Effects in Hybrid Nanostructures. This MURI began in FY12 and was awarded to a team led by Professor Naomi Halas at Rice University. This MURI is investigating nanomaterials and how these materials can control the propagation of electromagnetic (EM) energy.

Fundamental research involving metamaterials, quantum dots, plasmonic nanostructures, and other materials systems during the last decade has demonstrated the unique ability to selectively and actively control and attenuate electromagnetic energy from the far infrared (IR) through ultraviolet (UV) regions. The absorption frequency is dependent on shape, size, orientation, and composition of the nanomaterial. The nanoparticles act as antennae that redirect, focus or otherwise re-radiate the incoming energy. Because this is a resonance phenomenon, the media is generally transparent over a broad frequency range, with one or more resonances that absorb at specific frequencies. A goal in the control of the propagation of EM energy is the design of a material that absorbs over a broad frequency range and is transparent at one or more specific frequencies.

The objective of this research is to develop a fundamental understanding of nanomaterials to control the propagation of EM energy, with a particular emphasis on designing and investigating materials that have a broad spectrum absorption with a narrow, selective window of transmission. The MURI team is using a combination of computational, nanoscale fabrication, and characterization techniques to tailor electromagnetic properties for materials in specific, selected regions of the spectrum. The research team is focusing on designing, synthesizing, and combining nanoparticles and nanoparticle-based complexes to yield nanocomplexes exhibiting optimized coherent effects. This research may ultimately enable the design of materials with precisely-positioned transparency or absorbency windows that will impact Army applications in broadband scattering and absorption.

6. Theory and Experiment of Cocrystals: Principles, Synthesis and Properties. This MURI began in FY13 and was awarded to a team led by Professor Adam Matzger of the University of Michigan at Ann Arbor. This MURI team is investigating molecular co-crystal formation and the implications for controlling solid-state behavior. This research is co-managed by the Chemical Sciences and Materials Science Divisions.

The largely untapped potential for creating new molecular crystals with optimal properties is just beginning to be realized in the form of molecular co-crystallization. Co-crystallization has the potential to impact the macro-scale performance of many materials, ranging from energetic materials, to pharmaceuticals, to non-linear optics. Unfortunately, the dynamics of molecular co-crystal formation is poorly understood. Molecular co-crystals contain two or more neutral molecular components that rely on non-covalent interactions to form a regular arrangement in the solid state. Co-crystals are a unique form of matter, and are not simply the result of mixing two solid phases. Organic binary co-crystals are the simplest type and often display dramatically different physical properties when compared with the pure 'parent' crystals. A significant amount of research on co-crystal design has been carried out by the pharmaceutical industry for the synthesis of pharmaceutical ingredients. However, co-crystal design has not been exploited in broader chemistry and materials science research areas. A recent breakthrough discovery demonstrates that co-crystallization can be used to generate novel solid forms of energetic materials.

The objective of this MURI is to develop a fundamental understanding of intermolecular interactions in the context of crystal packing, and to use the knowledge gained for the design of new co-crystalline molecular materials with targeted, optimized physical and chemical properties. In the long term, a better understanding and

[1] Shuman ES, Barry JF, DeMille D. (2010). Laser cooling of a diatomic molecule. *Nature*. 467:820–823.

control of molecular co-crystallization has the potential to improve the properties of a variety of materials, including: energetic materials, pharmaceuticals, organic semiconductors, ferroelectrics, and non-linear optical materials.

7. Artificial Cells for Novel Synthetic Biology Chassis. This MURI began in FY13 and was awarded to a team led by Professor Neal Devaraj at the University of California - San Diego. The goal of this MURI is to understand how biological and biomimetic synthetic cellular elements can be integrated to create novel artificial cells with unprecedented spatial and temporal control of genetic circuits and biological pathways. This research is co-managed with the Chemical Sciences Division.

The field of synthetic biology aims to achieve design-based engineering of biological systems. Toward this goal, researchers in the field are identifying and characterizing standardized biological parts for use in specific biological organisms. These organisms serve as chassis for the engineered biological systems and devices. While single-celled organisms are typically used as synthetic biology chassis, the complexity of even these relatively simple organisms presents significant challenges for achieving robust and predictable engineered systems. A potential solution is the development of minimal cells which contain only those genes and biomolecular machinery necessary for basic life. Concurrent with recent advances toward minimal biological cells, advances have also been made in biomimetic chemical and material systems, including synthetic enzymes, artificial cytoplasm, and composite microparticles with stable internal compartments. These advances provide the scientific opportunity to explore the integration of biological and biomimetic elements to generate an artificial hybrid cell that for the first time combines the specificity and complexity of biology with the stability and control of synthetic chemistry.

The objective of this MURI is to integrate artificial bioorthogonal membranes with biological elements to create hybrid artificial cells capable of mimicking the form and function of natural cells but with improved control, stability, and simplicity. If successful, these artificial cells will provide a robust and predictable chassis for engineered biological systems, addressing a current challenge in the field of synthetic biology that may ultimately enable sense-and-respond systems, drug-delivery platforms, and the cost-effective production of high-value molecules that are toxic to living cells (e.g., alternative fuels, antimicrobial agents).

8. Attosecond Electron Dynamics. This MURI began in FY14 and was awarded to a team led by Professor Stephen Leone at the University of California - Berkeley. The goal of this MURI is to use attosecond light pulses to study the electron dynamics of atoms and small molecules. This research is co-managed with the Physics Division.

Attosecond dynamics is a new field of scientific investigation which allows one to examine dynamics phenomena on the natural timescale of electronic processes in atoms, molecules, and materials. The timescale of microscopic dynamics in quantum systems occur at a timescale about one order of magnitude less than those for less-energetic processes, such as valence electronic transitions in molecules and semi-conductor materials. A recent scientific breakthrough known as double optical gating has lead to the production of broadband laser pulse widths as short as 67 attoseconds, making direct observation of a variety of electronic phenomena possible in real time. Thus, now there exist opportunities to examine a variety of electron-dynamics phenomena that arise from electronic motions in molecules on the attosecond timescale.

The objective of this research is to harness attosecond pulses of electromagnetic energy to probe matter (e.g., atoms, molecules, plasmas) at attosecond time scales for the real-time observation, control, and understanding of electronic motion in atoms, molecules, and materials. If successful, this research may lead to new synthesis methods, such as plasmonically-enhanced catalysis for the direct reduction of CO_2 to create fuels, new schemes and manufacturing methods for solar photovoltaics, nano-catalysts for fuel combustion, and high-density specific impulse propellants.

9. Multistep Catalysis. This MURI began in FY14 and was awarded to a team led by Professor Shelley Minteer at the University of Utah. The goal of this MURI is to enable multi-step chemical reactions through the rational design of architectures that control the spatial and temporal pathways of precursors, intermediates, and products. This research is co-managed with the Materials Science Division.

The Krebs cycle is an exquisite example of a regulated enzyme cascade which biological systems use to precisely control charge and reactant transport to produce energy for the cell. Conversely, man-made systems typically involve a series of conversions with intermediate purification steps to achieve a desired product, with yield losses that compound with each step. The current approach to achieve multi-step reactions in a single reactor is an arbitrary combination of multiple catalysts that is likely to lead to poor yield with unreacted intermediates or byproducts of reactants that have reacted with the incorrect catalysts. Recent breakthroughs in materials synthesis, such as self-assembly and lock-and-key type architectures, offer control of surface arrangement and topology that enable a much more effective approach to achieving multi-step reactions through control of spatial and temporal transport of reactants, electrons, intermediates, and products.

The objective of this research is to establish methodologies for modeling, designing, characterizing, and synthesizing new materials and structures for the design and implementation of multi-step catalysis. In particular, integrated catalytic cascades will be created from different catalytic modalities such that novel scaffolding and architectures are employed to optimize selectivity, electron transfer, diffusion, and overall pathway flux. If successful, this research will provide unique paradigms for exploiting and controlling multistep catalysis with dramatically enhanced efficiency and complexity. In the long term, the results may lead to new energy production and storage technologies.

10. Multi-Scale Responses in Organized Assemblies. This MURI began in FY15 and was awarded to a team led by Professor Sankaran Thayumanavan, at University of Massachusetts - Amherst. The goal of this MURI is to understand how a molecular level detection can be propagated across a macroscopic material to affect a global property change that spans multiple length and time scales, and connecting these multi-scale events to realize signal amplification. This research is co-managed with the Materials Science Division.

Living systems are complex systems capable of receiving and using information, interacting with each other and their environment, and performing specific functions in response to stimuli occurring at multiple length and time scales. These sophisticated, innate behaviors are essential for survival, and can be extremely valuable in non-natural systems. A variety of synthetic systems have been engineered to respond to specific stimuli; however, the dynamics of the chemical and material processes and interactions occurring at multiple length and time scales throughout the signal-propagate-response pathway are inadequately understood to rationally design autonomous, "living" systems. The daunting challenge toward synthetic "living" systems is predictably propagating a molecular level change, generated through the selective sensing of a trigger, into a readily discernible macroscopic change in a material's fundamental properties. This can only be addressed by developing a fundamental understanding of the chemical processes that occur at multi-scale levels – from molecular to nano to macroscopic length scales and from nanoseconds to hours. The inherent complexity involved in connecting these length scales, and the propagation and amplification of the resulting signals, requires a cohesive, multidisciplinary approach.

The integrated research plan led by Professor Thayumanavan is comprehensive and addresses each of the key elements needed to understand the fundamental multi-scale responses of adaptive systems occurring across length and time scales. The research is exploiting a variety of material platforms/approaches, including liquid crystal orientation, responsive amphiphiles, depolymerization, and biological/abiological composites with non-equilibrium molecular release to address propagation and amplification at multiple length scales. Each system approach is innovative, well-formulated, and focused on a complete understanding of the basic research principles controlling each approach. A variety of triggers will be considered throughout the effort including pH, temperature, redox, light, and enzymes. A key part of this effort is the ability to monitor dynamic changes during the cooperative reorganization processes at the interface, and this is addressed by integration of novel characterization techniques such as in situ liquid cell transmission electron microscopy. If successful, this fundamental research may ultimately enable Army-relevant technologies in stimuli-responsive systems such as self-decontaminating materials, controlled release for hazardous materials management or drug delivery, and responsive systems for self-healing and smart materials.

C. Small Business Innovation Research (SBIR) – New Starts

Research within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. The Division did not have any new-start SBIR contracts in FY15; however, the Division managed active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY15 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY15, the Division managed six new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of three Phase I contracts and three Phase II contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY15 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY15, the Division managed two new ARO (Core) HBCU/MI projects and 11 new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The PECASE winners for each year are typically announced by the White House at the end of the calendar year. However, the FY13-FY15 PECASE recipients had not yet been announced by the end of FY15. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY15, the Division managed 11 new DURIP projects, totaling $1.9 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. University Affiliated Research Center (UARC): Institute for Soldier Nanotechnologies (ISN)

The ISN, located at the Massachusetts Institute of Technology (MIT), carries out fundamental, multidisciplinary, nanoscience research that is relevant to the Soldier. Nanoscience research creates opportunities for new materials, properties, and phenomena as material properties (*e.g.*, color, strength, conductivity) become size dependent below a critical length scale of about 500 nanometers. The research performed at the ISN falls into five Strategic Research Areas (SRAs): (i) Lightweight, Multifunctional Nanostructured Materials (ii) Soldier Medicine, (iii) Blast and Ballistic Threats, (iv) Hazardous Substances Sensing, and (v) Nanosystems Integration. Each SRA is further divided into research themes. Detailed descriptions of each SRA and its corresponding themes are available at the ISN program website (http://mit.edu/isn/research/index.html).

In FY15, the ISN supported 41 faculty, 70 graduate students, and 28 postdoctoral fellows across 17 departments at MIT. The ISN program is unique in that it currently has 12 industrial partners positioned to receive promising technical results and work to bring new products and capabilities to the Soldier, as well as a mechanism for additional industry partners to join and leave the Institute, depending on needs and activities. A U.S. Army Technical Assessment Board and an Executive Steering Board annually review the ISN research portfolio, assessing the goals of the various projects and research results. The ISN and its industry partners are wellsituated to perform basic and applied research in response to Soldier needs now and in the future. A total of $7.9 million of program funds was allocated to the ISN in FY15, which was the third year of a contract that was renewed in FY12 for a five-year period. Of these FY15 funds, $6.5 million was allocated for 6.1-basic research and $1.4 million was allocated for five applied-research projects, including three new projects.

I. DARPA Biofuels Alternative Feedstocks

The Biofuels Alternative Feedstocks program is developing affordable alternatives to petroleum-derived jet fuels (JP-5, JP-8) using algae. The Division's Electrochemistry program manger aids in the management of this this DARPA program. DARPA seeks to conduct a one-year demonstration of state of the art algae oil production to determine current economic maturity.

J. DARPA Agnostic Compact Demilitarization of Chemical Agents (ACDC) Program

DARPA's Agnostic Compact Demilitarization of Chemical Agents (ACDC) program is exploring new technologies for neutralization of bulk stores of chemical warfare agents (CWAs) and organic precursors at or near the site of storage. ACDC is developing and demonstrating the technologies needed to construct a transportable, prototype system that converts organic compounds into constitutive carbon/nitrogen/phosphorous/sulfur oxides and stable alkali or alkaline earth metal salts, or another demonstrated safe form. A final ACDC system would feature chemistries for agent destruction and sequestration of halogens and other components using locally available resources. ARO is providing subject matter exptertise and an ARO program manager is serving as the COR on the awarded efforts.

K. DARPA Make-It Program

The DARPA Make-It program aims to address these challenges by developing technologies to accelerate chemical discovery and production beyond conventional batch-based capabilities by exploiting continuous synthetic approaches. The goal of Make-It is to develop a fully automated chemical synthesizer that can produce, purify, characterize and scale a wide range of small molecules. Make-It systems would likely include components for knowledge-based computational tools for reaction pathway prediction; algorithms for automation and process control; and interconnected fluidic modules for continuous synthesis, in-line characterization, purification and formulation. If realized, such a system would not only speed the pace of chemical innovation and small-molecule manufacturing, but would also provide an accessible chemical synthesis platform for non-specialists. ARO is providing subject matter exptertise and an ARO program manager is serving as the COR on the awarded efforts.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Chemical Sciences Division.

A. Chemical Transformations via Photon Induced Metal-to-Molecule Electron Transfer

Professor Phillip Christopher, University of California, Riverside, YIP Award

The objective of this research is to manipulate selectivity in heterogeneous catalytic reactions on metal nanoparticles, by using light to direct the conversion of reactants into desired products. Central to this objective is understanding how photons interact with bonds formed between metal active sites and adsorbed species. The PI has identified resonant electronic transitions localized at Pt-CO interfaces on small Pt nanoparticles, and showed that resonant photoexcitation of Pt-CO bonds allowed control of selectivity in the preferential oxidation of CO in H_2 rich environments. This demonstration represents an important finding, and raises questions regarding which Pt-CO bonds were being activated with light. When metal catalysts are deposited on oxide supports they exist in a variety of geometries, ranging from single metal atoms to 3D particles (see FIGURE 1). The distribution of structures creates a distribution of metal sites that molecules can bond with, each having varying catalytic functionality. It is critical to identify which bonding sites were involved in our demonstrations of light induced control of reaction selectivity, to enable optimization of our ability to control how light interacts with catalytic processes.

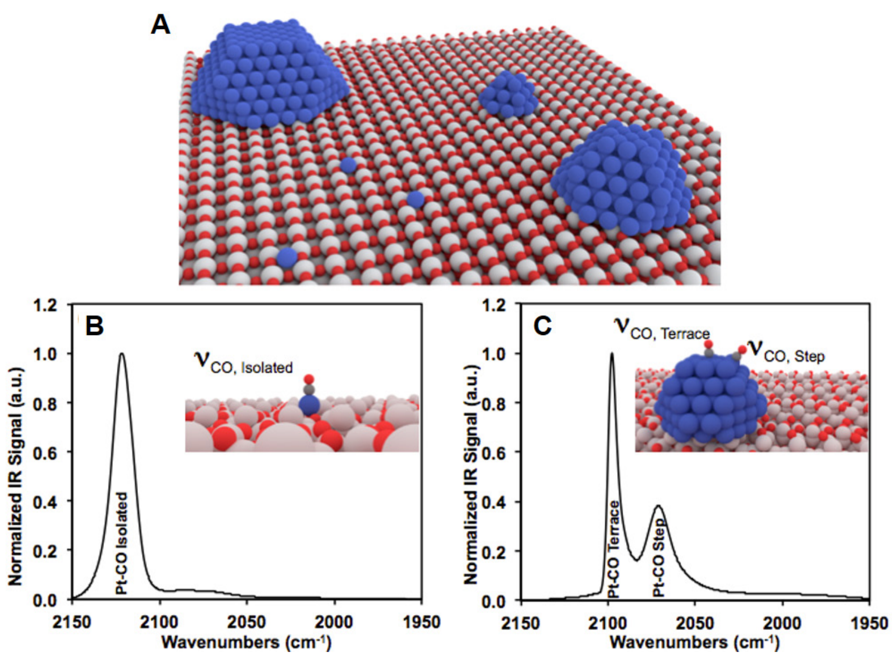

FIGURE 1

Identification of active Pt catalytic sites for CO chemisorption and oxidation. (A) Schematic of various Pt nanostructures deposited on prototypical oxide support. (B) FTIR spectrum of CO chemisorbed to isolated Pt atoms on a TiO_2 support. Inset shows the assigned geometry. (C) FTIR spectrum of CO bound to small Pt nanoparticles on Al_2O_3. Inset shows geometric structures assigned to the observed CO stretches.

In order to probe how light is interacting with various geometries of Pt-CO bonds a site specific characterization approach was needed. The PI and coworkers utilized careful synthetic protocols to vary the concentration of different potential CO bonding sites (isolated Pt atoms on oxide supports, well-coordinated Pt atoms at terraces on nanoparticles and under-coordinated Pt atoms at steps and defects on nanoparticles) and probed the interaction of CO with these different Pt sites using high-resolution diffuse reflectance FTIR spectroscopy (DRIFTS). The highlights of these results are shown in FIGURE 1B-C, where DRIFT spectra of CO bound to the various Pt sites are shown. It is clearly seen that through careful sample preparation and measurements we can differentiate between CO bound to different Pt sites on oxide-supported Pt catalysts.

With rigorous spectral assignments for CO adsorbed at various Pt sites the PI and coworkers sought to (i) probe whether Pt catalysts restructure under CO oxidation reaction conditions and (ii) compare the reactivity of CO adsorbed to different Pt sites. To analyze restructuring of Pt catalysts, Pt nanoparticles of varying size (no single Pt atoms on the oxides are present) on Al_2O_3 supports were synthesized. The Pt surfaces at room temperature were saturated with CO, a DRIFT spectrum collected, the catalyst raised to CO oxidation reaction conditions (1%CO, 1%O_2, 98% He at ~170 °C) and a DRIFT spectrum collected, next the catalyst was coolec back to room temperature and a DRIFT spectrum collected of a CO saturated surface (see FIGURE 2A). They performed the identical experiment for 4 Pt particle sizes and utilized peak de-convolution, integration and extinction coefficients to quantify the concentration of well- and under-coordinated Pt atoms at the surface of Pt nanoparticles. The results demonstrated that, compared to geometric model predictions, Pt nanoparticles reconstruct at room temperature due to CO adsorption, and reconstruct even further under reaction conditions (see FIGURE 2B). The reconstruction roughens the Pt nanoparticle surfaces, creating higher density of under-coordinated Pt atoms. These results represent the first measurements of adsorbate-induced reconstruction of Pt nanoparticles that provide quantitative analysis of surface roughening and provide important insight regarding the catalytic sites that are present under reaction conditions. Further, the Christopher lab utilized the rigorous spectral assignments in FIGURE 1 to directly compare the reactivity of CO bound to isolated Pt atoms, CO bound to metallic Pt atoms at nanoparticle surfaces and CO bound to oxidized Pt clusters. This was executed using time-resolved DRIFTS that enabled them to identify that the reactivity of CO significantly depends on the nature of the Pt site it is bound to (see FIGURE 2C). Furthermore this is the first direct demonstration that isolated, un-promoted Pt atoms on oxide supports are more reactive than Pt nanoparticles for the CO oxidation reaction.

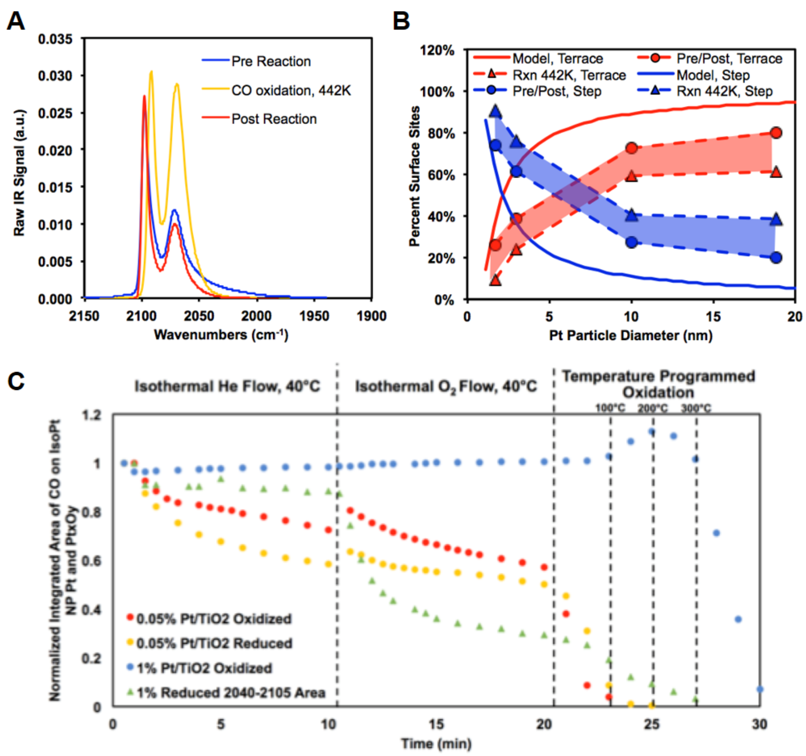

FIGURE 2

***In-situ* analysis of adsorbate induced Pt nanoparticle restructuring and site-specific measurements of CO oxidation reactivity.** (A) DRIFT spectra of saturated CO monolayers on 19 nm Pt particles at room temperature pre-reaction, under reaction conditions and post reaction. An obvious reconstruction is observed. (B) Quantified fraction of Pt sites existing as well-coordinated terrace sites and under-coordinated step sites as a function of particle size, predicted from classic models, measured at room temperature and measured under reaction conditions. Significant deviations from the model predictions demonstrate the restructuring. (C)

Quantified CO concentration on various Pt active site geometries during during isothermal and temperature programmed oxidation demonstrating that CO on isolated Pt atoms is highly active for CO oxidation.

B. Polymers that Depolymerize from Head-to-Tail in the Solid State
Professor Scott Phillips, Pennsylvania State University, Single Investigator Award

Polymers have traditionally been designed for static materials that last indefinitely. The objective of Professor Phillips' research is to develop new classes of polymers that retain the desired features of resilience, but also impart polymeric materials with the ability to respond to their surroundings in ways that are dynamic, purposeful, and functional, much like materials in living systems. More specifically, this effort seeks to develop polymers that depolymerize in the context of solid-state materials when triggered by specific applied stimuli. The ideal design enables facile tuning of the stimulus to which the polymers respond, as well as high specificity for a desired stimulus. Moreover, access to several classes of these polymers will facilitate tuning of the rates of response (via the rates of depolymerization) and global structural properties of the materials. Research efforts in FY15 resulted in the design of a new polymer that depolymerizes in the solid state and the development of a general strategy for rendering detection units accessible at the interface of a solid plastic and a surrounding medium. This general strategy enables solid-state depolymerization of polymers that previously were resistant to depolymerization. These types of polymers should enable (i) efficient, low-energy methods for recycling and/or disposing of plastics; (ii) plastics that disappear (i.e., convert to small molecules or gas when triggered); (iii) soft materials that reconfigure themselves and their function/structure in response to their environments; and (iv) polymeric materials that offer multiple, simultaneous capabilities (such as a sensor and a structural material). To that end, in FY15 Professor Phillips' group also demonstrated applications of solid-state depolymerization in the context of low-energy recycling strategies for polymeric materials as well as adhesives that are de-bonded selectively in response to specific applied signals.

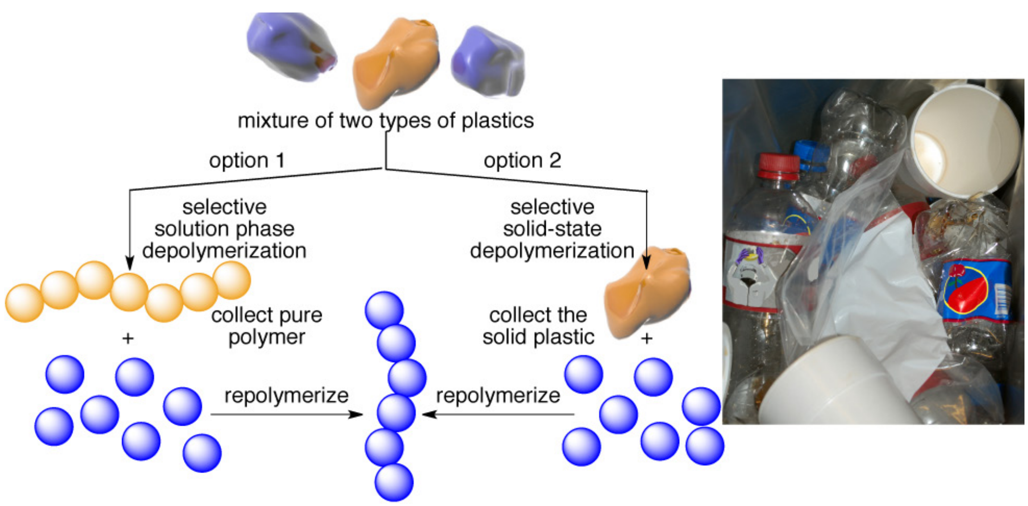

FIGURE 3

Strategies for recycling polymeric materials made from depolymerizable polymers. Self-immolative poly(benzyl ethers) were used in this research to demonstrate selective, programmed, room-temperature, and continuous depolymerization of plastics to monomers when the plastic is no longer needed.

C. Energetic – Energetic Cocrystals of Diacetone Diperoxide with Trihalotrinitrobenzenes
Professor Adam Matzger, University of Michigan, MURI award

In a molecular crystal, there is a regular arrangement of molecules characterized by a unit cell, symmetry of the packing, and a host of intermolecular interactions. Such order is also present in cocrystals, with two or more molecular species occupying the unit cell. Cocrystallization has the potential to improve the properties of a variety of materials, including explosives, ferroelectrics, and second harmonic generators. Because of their mixed chemical composition, cocrystals behave differently than pure crystals, particularly in ways that can be exploited for improved materials. In this research, the PI and coworkers show that the properties of diacetone diperoxide, a sensitive explosive with low density and low explosive velocity, can be dramatically improved through co-crystallization with selection of the proper energetic molecule co-former. In particular, it was shown for the first time that two explosives with high sensitivity can cocrystallize to form an explosive with dramatically lower sensitivity than the parent compounds. This is a unique and unprecedented observation of sensitivity enhancement in the field of energetic cocrystals research.

In this work, diacetone diperoxide (DADP) was cocrystallized with each of 1,3,5-trichloro-2,4,6-trinitrobenzene (TCTNB), 1,3,5-tribromo-2,4,6-trinitrobenzene (TBTNB), and 1,3,5-triiodo-2,4,6-trinitrobenzene (TITNB) to form three distinct 1:1 mole ratio cocrystalline materials (see FIGURE 4). The resulting cocrystals combine DADP, an easily synthesized explosive with high sensitivity, low density, and high volatility, with trihalonitrobenzenes which offer high density and low volatility. The cocrystal structure of DADP/TCTNB (cocrystal **1**) is shown FIGURE 5.

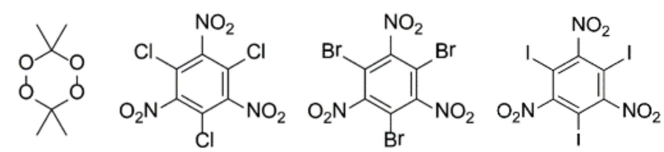

FIGURE 4

The molecular structures of DADP, TCTNB, TBTNB, and TITNB. The cocrystal structures of DADP/TCTNB (cocrystal **1**) and DADP/TBTNB (cocrystal **2**) are very similar.

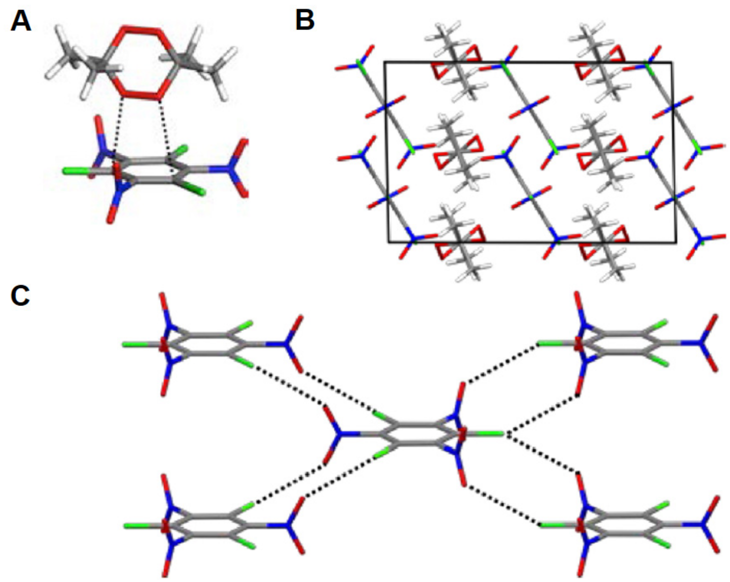

FIGURE 5

Cocrystal structure of (1). (**A**) Peroxide-aromatic ring interaction, (**B**) unit cell, and (**C**) chlorine-nitro interactions.

The molecular cocrystal of DADP with TITNB (cocrystal **3**) was synthesized by solvent mediated transformation of the parent compounds in acetonitrile. Notably, the cocrystal **3** is not isostructural to cocrystals **1** and **2**. The cocrystal **3** features a novel halogen-peroxide bonding interaction which is absent in **1** and **2**. In cocrystal 3, the peroxide functional group interacts with an iodine atom of TITNB (see FIGURE 6). This is the first observation of a halogen-peroxide intermolecular interaction. This contrasts with cocrystals **1** and **2** where the peroxide group interacts with the electron deficient aromatic rings of TCTNB and TBTNB. These intermolecular differences between **3** and cocrystals **1** and **2** lead to dramatic differences in properties.

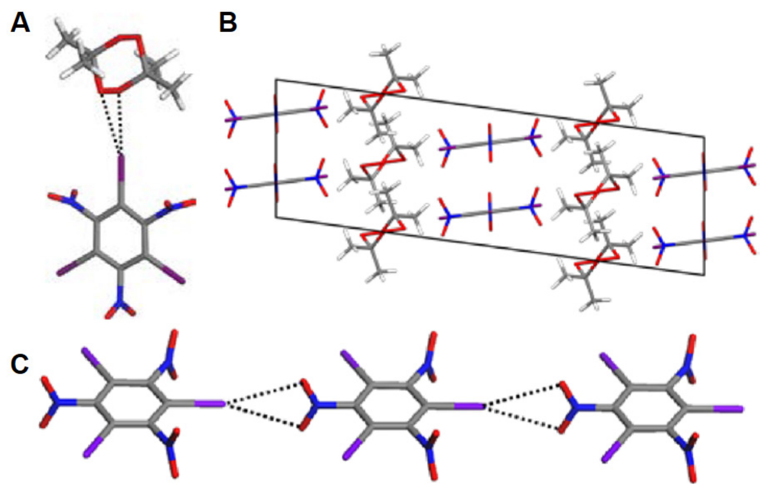

FIGURE 6

Cocrystal structure of (3). (A) Peroxide-idodine interaction, 2.95 Å (B) unit cell, and (C) iodine-nitro interactions.

A key property of any energetic material is sensitivity. Impact sensitivities were measured for each of the pure solids and for cocrystals **1** and **3** (see FIGURE 7).

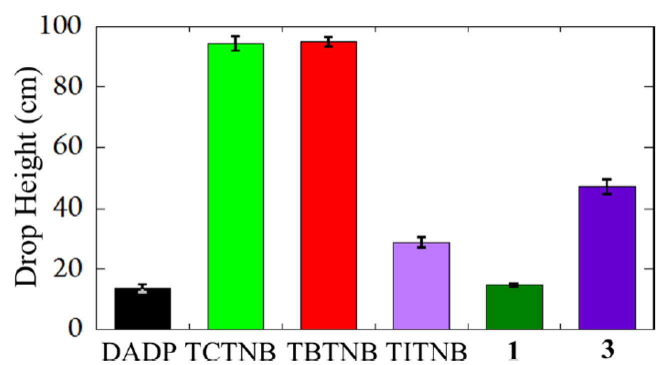

FIGURE 7

Relative impact sensitivity of explosive pure solids and cocrystals as $h_{50\%}$.

DADP is known for having a high sensitivity. Each of the trihalonitrobenzenes exhibit lower sensitivity than DADP, with TITNB exhibiting an unexpectedly high sensitivity as compared to the chloro and bromo derivatives. Cocrystal **3** possesses sensitivity far lower than either of its parent compounds DADP or TITNB, an unprecedented observation. This result is the first example of two relatively high-sensitivity explosives synergistically stabilizing each other via intermolecular interactions in a solid co-crystalline state to form a new explosive with dramatically reduced sensitivitiy. Note that cocrystal **1** has the same high sensitivity as the parent DADP compound, and that **1** is lacking the halogen-peroxide interaction that is present in **3**.

D. Multifunctional Integrated Fabrics

Professor Yoel Fink, Massachusetts Institute of Technology, UARC-ISN

The goal of this research is to enable next generation fiber functionality for multifunctional active fabrics by harnessing newly discovered multi-material in-fiber fluid instabilities and use the resultant knowledge to develop new understanding of basic science and engineering of nanoparticles. Under this project scientists are harnessing non-linear effects to produce "fiber capillary breakup" localized domains in an otherwise continuous fiber and to demonstrate the ability to generate millions of discrete devices in a fiber. The major accomplishments on this project in the past year include applying multi-core fiber drawing and selective breakup method to fabricate an integrated optoelectronic device that is composed of Ge and Pt in silica clad fiber (see FIGURE 8); and designing and successfully drawing a fiber structure at various scales that contained a semiconductor core (amorphous chalcogenide glass) flanked by two electrodes (conductive polyethylene) in polycarbonate cladding (see FIGURE 9).

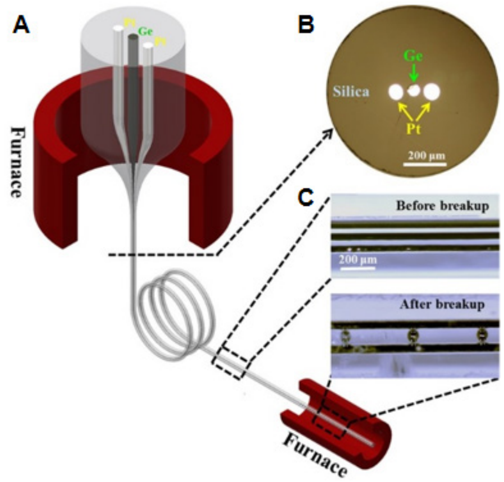

FIGURE 8

Fabrication process. (A) Schematic representation of the thermal drawing of a triple-core fibre and after-draw selective breakup process in a heating furnace. (B) Optical microscope image of the obtained fibre cross-section. The resulting silica-cladding fibre has three cores: one semiconductor (germanium) core in the middle and surrounded by two metal (platinum) cores. (C) Side views of the triple-core fibre before and after the selective breakup process.

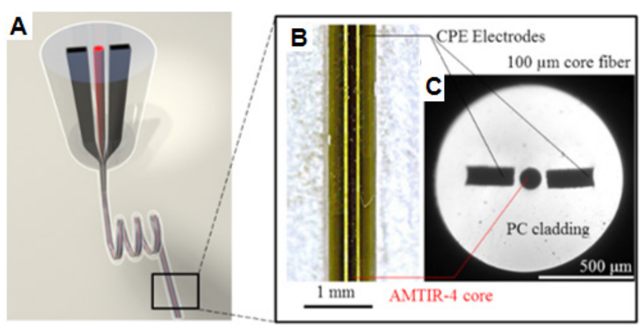

FIGURE 9

Fiber draw schematics. (A) Schematic representation of the thermal draw of a triple core fiber. Cladding of the fiber is Polycarbonate, the middle core is chalcogenide semiconductor As_2Se_5, and the outer two cores are polymeric electrodes. The distance between the cores was intentionally chosen so that a contact will be formed between the core and the electrodes upon induction of selective break-up. (B) Optical microscope image of the obtained fiber (core diameter ~100 µm) – axial and cross sectional views. (C) The fiber drawn is redrawn again to reduce the dimensions of the constituents, electrode extensions are added to facilitate integration with the fiber.

D. Reactive Chemical Species Stabilization and Fundamental Studies of Small-Molecule Reactivity in Metal-Organic Frameworks

Professor T. David Harris, Northwestern University, YIP Award

The goal of this research is to design and synthesize porphyrin containing Metal-Organic Frameworks (MOFs) and study their ability to stabilize small reactive molecules as well as their stability and reactivity in catalytic transformations. MOFs were chosen as a scaffold because 1) their rigid structure provides a surface upon which to anchor reactive chemical species, precluding participation in side reactions typically observed in molecular catalysts; and 2) their solid-state composition enables gas-phase reactions in absence of solvent. Previous work demonstrated a five-coordinate porphyrin iron-dioxygen adduct embedded within a MOF scaffold, PCN-224FeO$_2$, the first structurally characterized example of any five-coordinate iron-dioxygen species (see FIGURE 10). This initial study successfully demonstrated the ability of MOFs to act as solid-state scaffolds for the stabilization of reactive chemical species.

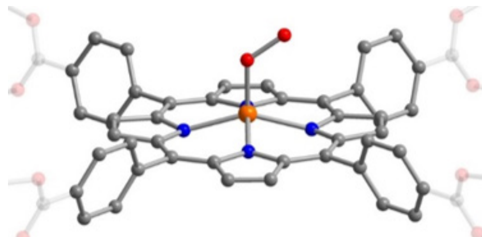

FIGURE 10

Crystal structure of PCN-224FeO$_2$. Green, orage, red, blue, and gray spheres represent Zr, Fe, O, N, and C atoms, respectively.

In FY15, the research team extended their investigations to iron nitric oxide chemistry. Heme dinitrosyl adducts have been previously studied in model systems, but their stereochemistry has yet to be validated. As an alternative to using molecular systems to probe the stereochemistry, Professor Harris has utilized heme-containing MOFs to isolate these species. A single crystal of PCN-224Fe(II) was exposed to 1 atmosphere of NO and subsequently cooled to -78°C. Single-crystal X-ray diffraction analysis was consistent with the dinitrosyl adduct, PCN-224Fe(NO)$_2$, and represented the first structurally characterized porphyrin trans-dinitrosyl complex. Mossbauer spectra for both the mono- and di-nitrosyl complex were consistent with previously reported values for five coordinate pophyrin $\{FeNO\}^7$ complexes and supported the formation of dinitrosyl complex, respectively.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Integrated Multi-Scale Approach For Understanding Ion Transport In Complex Heterogeneous Organic Materials

Investigators: Professors Andrew Herring, and Daniel Knauss, Colorado School of Mines, MURI Award
Recipient: ProtonOnSite

Professor Herring's team recently discovered anion exchange membranes with very high hydroxide conductivity and stability (see FIGURE 11). Even at 50% RH the material has a hydroxide conductivity >50 mS cm^{-1}, making these materials attractive for commercialization. This behavior is because the hydroxide anion moves via a Grotthus hoping mechanism rather than via a vehicular mechanism, in deed the activation energy for water diffusion in these materials is twice that for hydroxide conductivity. The swelling from water vapor is minimal and even from liquid water is half that of a typical proton exchange membrane. The materials are tough due to the nature of the cross linking that occurs during thermal processing and the films can be made as thin as 20 µm. Anion exchange membranes have the potential to completely change electrolysis for hydrogen production or for the production of electrofuels such as ammonia as the catalysts are non-precious metals. ProtonOnSite is evaluating these membranes for commercial applications in electrolyzers.

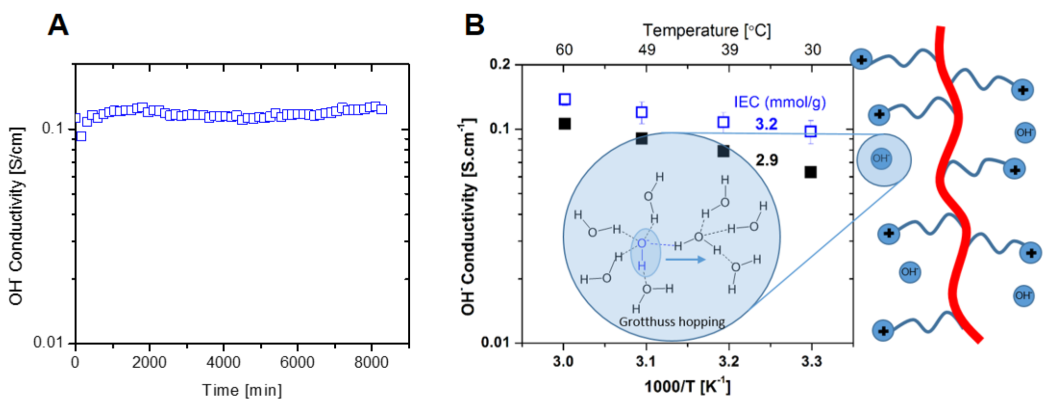

FIGURE 11

Hydroxide xonduxtivity data for a polyphenylene oxide-b-polyvinylbenzyltrimethylamine polymer. (A) Stability data at 95% TH and 60°C; (B) data for two IECs of the polymer at 95% RH with a representation of the Grotthus hoping of hydroxide.

B. Coherent Effects In Hybrid Nanostructures For Lineshape Engineering Of Electromagnetic Media

Investigator: Professor Naomi Halas, Rice University, MURI Award
Recipient: U.S. Army Edgewood Chemical Biological Center (ECBC)

The objective of this multidisciplinary research, led by Professor Halas, is to functionalize nanoparticles to control the optical and electromagnetic properties of plasmonic and plexcitonic nanostructures as an approach to propagate electromagnetic energy. Professor Halas and her team have been focusing on the synthesis of novel complexes and mixtures including doped Si nanocrystals, hedgehog nanoparticles, and gold nanorod/B-doped silicon nanocrystal mixtures to engineer transparency windows in an extinction resonance lineshape. In FY15, the team successfully created hedgehog nanoparticles made up of negatively charged carboxylate-terminated polystyrene microspheres on which positively charged ZnO nanoparticles were adsorbed. These unique nanoparticles demonstrate no aggregation and an extinction spectrum that has a tunable transmission window between 700-1100 nm depending on the geometry of the ZnO “spikes”. This significant finding may be a viable approach to easily disperse obscurants in both aqueous and non-polar organic solvents (see FIGURE 12). Recently, ECBC initiated a new effort with co-PI Nick Kotov to scale-up a variety of hedgehog particles which will be used in aerosolization studies at ECBC.

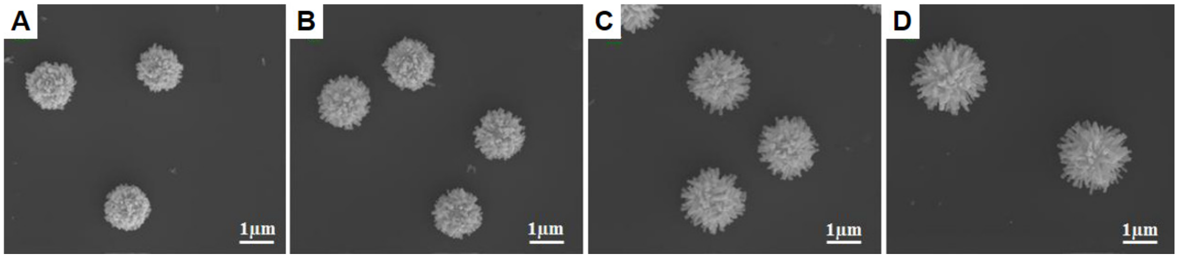

FIGURE 12

SEM images of hedgehog particles with different ZnO nanospike lengths. ZnO nanospike lengths in each panel are: (A) 0.19 mm; (B) 0.27 mm; (C) 0.4 mm, and (D) 0.6 mm.

C. Fractal Assembly of Polymeric Nanoparticles into Fibers versus Globules

Investigator: Professor Nicholas Leventis, Missouri University of Science and Technology, Single Investigator Award
Recipient: PM Soldier Protection and Individual Equipment, Technical Management Directorate

This objective of Professor Leventis’ research is to understand the molecular foundation of the macroscopic mechanical strength of nanostructured materials in an effort to control the 3D assembly of polymeric nanoparticles into nanofibrous aerogels. If successful, this research will provide a framework for the rational design of nanostructured polymeric materials with exceptional bulk mechanical properties. Research efforts in FY15 focused on gaining an understanding of and optimizing structure-property relationships of shape memory polyurethane aerogels which have demonstrated superelasticity - the ability to recover from extreme temperatures and stress deformations. Due to the potential utility of these materials in impact absorption, a panel of these materials was sent to the PM Soldier Protection and Individual Equipment, Technical Management Directorate (through a subcontract with the University of Texas at Dallas) for impact testing. The initial round of testing demonstrated that these shape memory aerogels had full recoverability, even after 10 rounds of testing. A second, larger panel of materials has been sent for subsequent testing. If successful, these materials have the potential to render new materials for use in Soldier head armor.

D. Quantum Control Research Leads to a Technology Transfer in the Pharmaceutical Industry

Investigator: Professor Herschel Rabitz, Princeton University
Recipient: Industry

ARO has funded basic science research for almost 30 years in the domain of controlling quantum dynamics phenomena, utilizing shaped laser pulses for that purpose. Quite surprisingly, this highly fundamental, long-term research area led to a technology transfer in FY15, due to relevance to a practical need in another domain lying within the pharmaceutical industry. The latter application in the pharmaceutical industry concerns the discovery of complex formulations for monoclonal antibody drugs. The family of monoclonal antibody drugs is the prime focus of many major pharmaceutical companies, especially in the oncology area. An acceptable formulation, containing the antibody along with other excipients, is essential for creating a final utilitarian drug product.

The disparity between the two seemingly different areas of quantum control and antibody formulation hides an important linkage, which in itself is of fundamental scientific importance. In particular, shaping laser pulses requires optimization of the physical objective over a large number of control field variables. In turn, discovering complex formulations for monoclonal antibodies has become a limiting factor in reaching clinical trials for cases requiring many excipients for a successful formulation. It was recognized that the latter problem can also be viewed in a control context where the desired property of the drug formulation is being optimized over the family of excipients. At a deeper level, the fields of quantum control and antibody formulations may both be expressed in terms of their respective control landscape, which is the physical objective as a function of the appropriate control variables. A fundamental part of this research is directed towards understanding the topology of such control landscapes, regardless of whether the variables are laser fields or chemical substituents (excipients). Under appropriate conditions, this landscape analysis led to the conclusion that optimization should be readily achieved despite the high dimensionality of the search space. A second factor contributing to this technology transfer was the development of a mathematical tool referred to as high dimensional model representation (HDMR), which is specifically directed at decomposing high dimensional functions (e.g., a control landscape) into a hierarchy of lower dimensional components, thereby greatly reducing the number of experiments required to explore the landscape. Thus, the technology transfer (carried out in cooperation with a major American pharmaceutical company) drew together basic scientific research supported by ARO in the domains of (i) control and (ii) mathematical function representation. The successful proof of principle experiments at the pharmaceutical company utilizing these latter basic research developments took a monoclonal antibody, which previously defied formulation (i.e., the number of apparent required experimental trials halted any attempt at finding a formulation), to now yield a formulation with excellent properties discovered with a very modest practical number of experimental trials.

The resultant technology transfer consists of an algorithm and associated software under license from Princeton University to a company for commercialization. Even at this early stage, wide interest is being shown by several major pharmaceutical companies. The product is expected to enable new drugs to reach clinical trial for testing and ultimately of public benefit. Thus, this technology transfer serves as a clear case of where basic research in one domain (quantum control) has led after many years of methodical advances to a high value application in a totally unanticipated domain (pharmaceutical development).

E. An Integrated Multi-Scale Approach For Understanding Ion Transport In Complex Heterogeneous Organic Materials

Investigator: Professor Andrew Herring, Colorado School of Mines,
and Professor E. Bryan Coughlin, U. Massachusetts - Amherst, MURI Award
Recipient: Kraton

Professor Herring's team now has a wide range of expertise in functionalizing polymers to act as anion exchange membranes. Working with Kraton we have synthesized the cationic form of their sulfonated pentablock material, Nexar (see FIGURE 13). The material is designed to be mechanically robust and to pahse sepeate to allow for rapid ion transport. There a number of unique properties, including that it will form 30 nm lamella, which will line up perpendicularly in a thin film, making this an ideal material for the electrode of an electrochemical device. Its water uptake is very low, yet it has a high water flux through the film. Kraton are actively perusing commercial applications of this material.

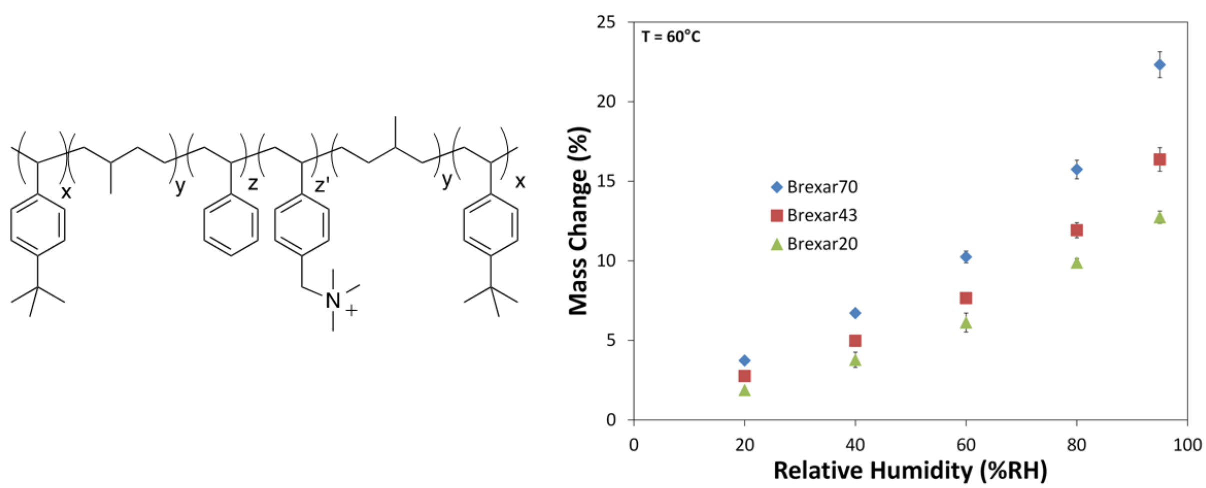

FIGURE 13

Cationic analogue of Nexar (Left) Structure (Right) water uptake at 60°C.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Single Molecule Resolution Of Immobilized Enzyme Function

Professor Joel Kaar, University of Colorado-Boulder, Single Investigator Award

The objective of this effort is to understand the connectivity between immobilized enzyme heterogeneity, substrate transport, and net reactivity of immobilized enzymes. This research will provide a more in depth analysis of protein-surface interactions at the molecular level, and investigate the distribution of folding states of enzymes covalently attached to a surface versus freely diffusing. Initial work in FY15 has focused on preparing different constructs of lipase containing sites for labeling and a unique peptide insert that can be used for immobilization (see FIGURE 14). Professor Kaar has demonstrated that enzyme variants can be site-specifically immobilized to functionalized silica nanoparticles while maintaining their activity.

In FY16, it is anticipated that the team will demonstrate how varying enzyme orientation and linker length impact heterogeneity in lipase structure and activity. The distribution in folding states of the variants upon surface immobilization will be measured using high-throughput single-molecule fluorescence resonance energy transfer (FRET). In addition, the impact of the underlying chemistry of the surface on this distribution will be investigated. Characterization of the heterogeneous structure and activity of immobilized enzymes using novel single-molecule biophysical tools will be used to develop immobilization strategies that improve function by reducing such heterogeneity. This effort will impact Army relevant areas including biotic-abiotic interfaces, biocatalysts, biosensors, and bioremediation.

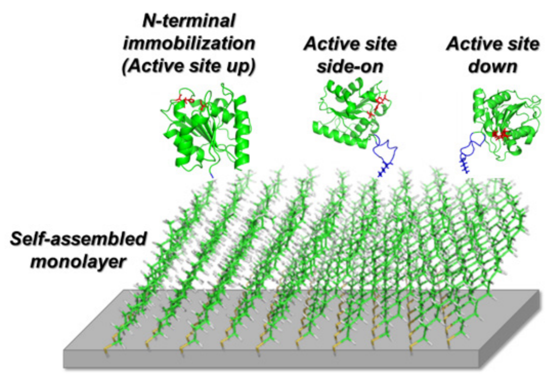

FIGURE 14

Site-specific immobilization of lipase variants with feasible orientations that can be investigated.

B. Highly Vibrationally Excited (v ≥ 4) H_2 Molecules by Stark-induced Adiabatic Raman Passage

Professors R. Zare and N. Mukherhee, Stanford University, Single Investigator and DURIP Awards

Diatomic hydrogen is the simplest molecule with just two electrons, both of which participate in the chemical bond. The vibrationally excited H_2 molecule has many important application in physics, astrophysics and chemistry. For example, it is known that the formation of H^- by the dissociative attachment of slow electrons ($H_2(v, J) + e \rightarrow H_2^- \rightarrow H^- + H$) is enhanced by 4 to 5 orders of magnitude by the vibrational excitation of H_2 within the ground electronic $^1\Sigma_g^+$ state. The very large cross-section for the formation of H^- from the v = 4 vibrational state of H_2 explained the anomalous density of H^- observed in a low-density hydrogen plasma. These ion sources are in turn essential to the development of high-intensity, high-brightness beams of neutral H atoms for their use in heating tokamak plasmas in fusion energy devices. However, populating the high vibrational levels of H_2 within the ground electronic state, which is the central task in preparing these sources, has never been done and is still considered to be an insurmountable challenge.

It is anticipated that in FY16 the research team will prepare a significant portion (greater than 50%) of the population of the ground (v = 0) vibrational state of H_2 or HD molecules in the vibrationally excited (v = 4) state using the Stark-induced adiabatic Raman passage (SARP) technique with a single-mode, nanosecond-pump pulse at 355 nm and a delayed single-mode Stokes pulse near 700 nm. In addition, the team will develop a suitable resonance-enhanced multi-photon ionization (REMPI) scheme for detecting the highly vibrationally excited level.

An experimental setup for preparing the HD (v=4) state using SARP with a 355 nm pump pulse and 696 nm delayed Stokes pulse is shown in FIGURE 15. The Spectra Physics injection seeded Nd^{+3}:YAG laser produces a second harmonic pulse at 532 nm and a third harmonic pulse at 355 nm from the fundamental Q-switched single mode pulse at 1064 nm. The energy of the 532 nm pulse is ~ 500 mJ, which is sufficient to pump a pulsed dye amplifier (PDA) generating an output pulse energy of ~ 40-50 mJ near 696 nm. The PDA is seeded with a frequency stabilized ring dye laser. The 40-50 mJ pulse energy at 696 nm provides the required fluence for the Stokes pulse. The 355 nm single mode pulse from the third harmonic of the YAG laser has an output energy ~ 300 mJ, which is more than sufficient to provide the pump pulse energy for the HD (v=4) excitation. The 355 nm pump pulse and the delayed 696 Stokes pulse are coupled by a beam-combiner before being focused into the molecular beam using a 60 cm focal length lens.

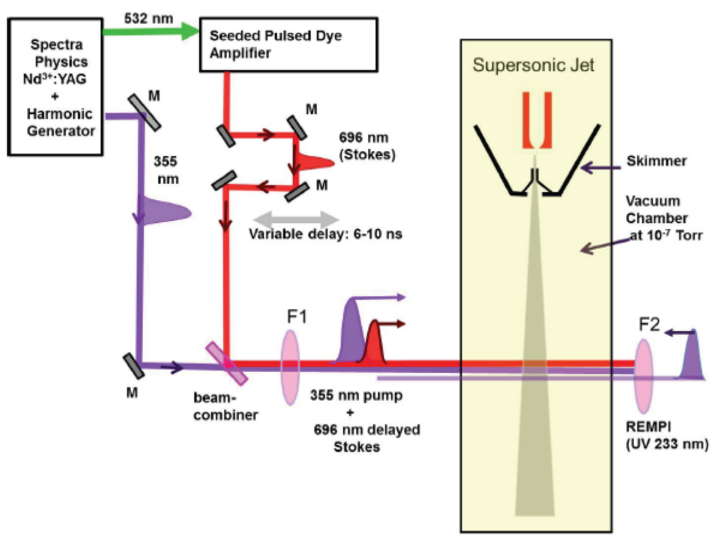

FIGURE 15

Schematic of the experimental setup for preparing the HD (v = 4) state using SARP with a 355 nm pump pulse and 696 nm delayed Stokes pulse with detection by REMPI.

C. Bio-inspired Design of Adaptive Catalysis Cascades

Professor Shelley Minteer, University of Utah, MURI Award
(Co-PIs P. Atanassov, University of New Mexico; S. Banta, Columbia University; S. Barton, Michigan State University; M. Sigman, University of Utah; I. Wheeldon, University of California - Riverside)

The objective of this MURI is to develop integrated catalytic cascades from different catalytic modalities such that novel scaffolding and architectures are employed to optimize selectivity, electron transfer, diffusion, and overall flux (see FIGURE 16). This research will create new hybrid inorganic, organic, and enzyme catalysts, create new materials for controlling electron transfer, and the diffusion of chemical species between catalyst sites, and create systems to physically isolate intermediates from the bulk environment. These novel technologies will generate new fundamental understanding of multi-step reactions of DoD interest. Initial work in FY15 was focused on developing the individual biological, organic, and inorganic catalysts that will be used for the hybrid catalytic cascades. Four enzyme systems (alcohol dehydrogenase, aldolase, oxalate oxidase, and oxalate decarboxylase) have been developed that will allow for easy immobilization on scaffolds, electrodes, etc. A library of over 25 TEMPO-type molecules have been synthesized for organoelectrocatalysis. Some of these are functionalized for utilizing click chemistry to bind to proteins or scaffolds and others are functionalized for forming redox polymers. Finally, a variety of manganese and platinum nanoparticle electrocatalysts for oxalate oxidation have been developed as inorganic electrocatalysts. Density functional theory calculations have been used to develop structure/function models and to predict properties before synthesis.

In FY16, it is anticipated that the team will be forming bi-catalytic and tri-catalytic cascades from these catalytic building blocks and studying the importance of spatial proximity. This research will provide a comprehensive understanding of the design constraints for these cascade materials.

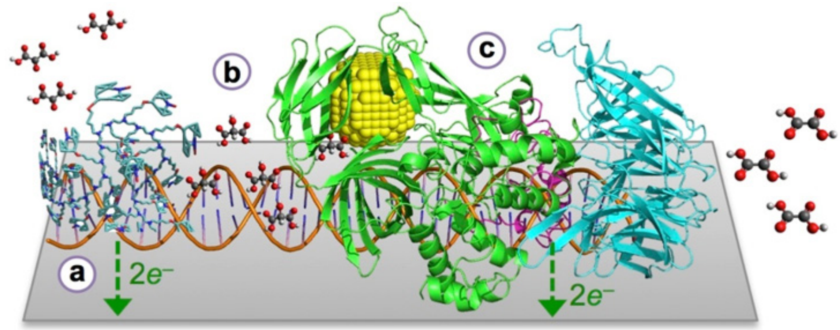

FIGURE 16

Hybrid tri-catalytic cascade of (A) organic catalyst, (B) inorganic nanoparticle catalyst, and (C) biological catalyst

D. Origami of Single Polymer Chains via Activated Permanent and Reversible Intra-chain Interactions

Professor Erik Berda, University of New Hampshire, Young Investigator Award

Professor Berda's research seeks to design and synthesize well-defined linear polymers that discreetly fold into architecturally defined 3D nanostructures and to establish a structure-property relationship for the resulting single-chain nanoparticles (SCNP). The current state of the art in SCNP synthesis involves linear polymer chains programmed to collapse using a single type of cross-linking reaction. Professor Berda's research is pushing beyond the current paradigm by exploring multiple, sequentially activated intra-chain interactions. This process is more akin to protein folding than previous examples of SCNP synthesis (albeit rudimentary when compared to biopolymers), and will lead to soft nanomaterials with well-defined structures and tunable properties (see FIGURE 17). Having recently demonstrated a variety of synthetic routes to functional SCNP using a number of intra-chain covalent and dynamic linkages, research plans in FY16 will focus on combining multiple intra-chain interactions into a single polymer system, a concept relatively unexplored outside of Professor Berda's research group. If successful, this work will render robust, yet adaptable nanostructured materials with utility in a number of areas including catalysis, sensing, self-healing and shape-programmable materials.

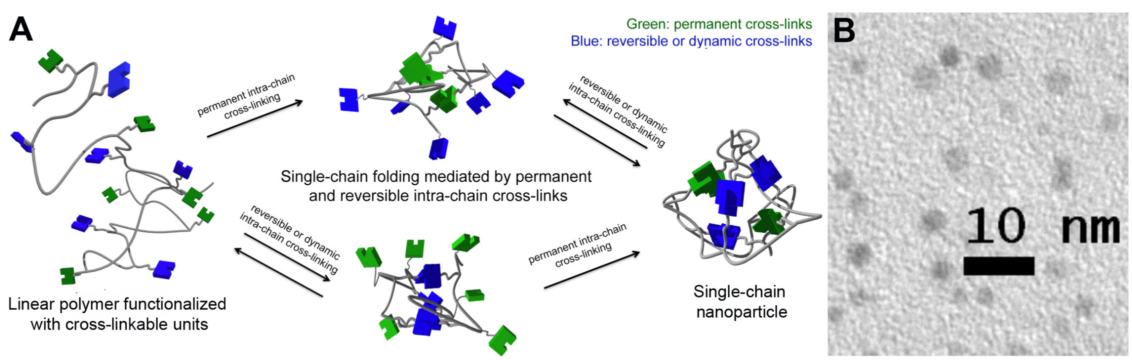

FIGURE 17

(A) Schematic representation of multifuctional SCNP synthesis and (B) representitive TEM image of SCNP made in the PI's laboratory.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Robert Mantz
Division Chief (Acting)
Program Manager, Electrochemistry

Dr. James Parker
Program Manager, Molecular Structure and Dynamics

Dr. Dawanne Poree
Program Manager, Polymer Chemistry
Program Manager (Acting), Reactive Chemical Systems

Ms. Wendy Mills
Contract Support, Reactive Chemical Systems

B. Directorate Scientists and Technical Staff

Dr. Douglas Kiserow
Director, Physical Sciences Directorate

Dr. Peter Reynolds
Senior Scientist, Physical Sciences Directorate

Dr. J. Aura Gimm
Program Manager, Institute for Soldier Nanotechnologies and Institute for Collaborative Biotechnologies

Dr. Kelby Kizer
Special Assistant to the Directorate Director

Dr. Larry Russell, Jr.
International Research Program Coordinator

Mr. John McConville
Technology Transfer Officer, Institute for Soldier Nanotechnologies

C. Administrative Staff

Ms. Wanda Lawrence
Contract Support

CHAPTER 4: COMPUTING SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2015* is to provide information on the programs and basic research supported by ARO in fiscal year 2015 (FY15), and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Computing Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY15.

A. Scientific Objectives

1. Fundamental Research Goals. The principal objective of the ARO Computing Sciences Division is to build the fundamental principles and techniques governing computational methods, models, and architectures to establish the foundation for revolutionary advances in intelligent, trusted, and resilient computing that provide increased performance and computational capability to enhance warfighter situational awareness, decision making, command and control, and weapons systems performance. More specifically, the Division supports basic research to establish new computing architectures and models for intelligent and trusted computing, to create novel data fusion and extraction techniques for efficient information processing, to create new capabilities in social informatics, and to build resilient computing systems for mission assurance. The results of these efforts will stimulate future studies and help keep the U.S. at the forefront of computing sciences research.

2. Potential Applications. Research efforts managed in the Computing Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. This program identifies and addresses the Army's critical basic research problems in the computing sciences where progress has been inhibited by a lack of novel concepts or fundamental knowledge. Computing science is pervasive in nearly all Army systems, particularly Command, Control, Communications, Computing, Intelligence, Surveillance, and Reconnaissance (C4ISR) systems. The number of information sources on the battlefield will grow rapidly; computing and information science research must provide the technology to process this in real-time and ensure that Soldiers and commanders do not experience information overload that could adversely affect their ability to make decisions. Also, in spite of the increased complexity of future battlefield information systems, dependence on them will only increase, therefore they must be extremely reliable and secure. Research in this program has application to a wide variety of developmental efforts and contributes to the solution of technology-related problems throughout the Army's Future Force operational goals. For this reason, computing science is a key technology underpinning future Army operations.

3. Coordination with Other Divisions and Agencies. The Division's research investment strategy is coordinated with partner disciplines and computer scientists at ARO, other directorates within ARL, other Army agencies, and related programs in other DoD and Federal organizations. The Division's research portfolio is supported by Army basic research Core funding with substantial additional resources from the Assistant Secretary of Defense for Research and Engineering [ASD(R&E)], including the Multidisciplinary University Research Initiative Program (MURI), and from other agencies, such as the Defense Advanced Research Projects Agency (DARPA).

To effectively meet Division objectives and to maximize the impact of potential discoveries for the Army and the nation, the Computing Sciences Division frequently coordinates and leverages efforts with Army scientists and engineers and with researchers in other DoD agencies. In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, interactions with the ARO Life Sciences Division include promoting research to investigate effective human-computer communication mechanisms and developing new metrics and benchmarks for social media analysis. The Division also coordinates efforts with the Network Sciences Division to explore new techniques for robust and resilient mobile ad hoc networks, to establish adversarial models for effective cyber defense, and to investigate fundamental principles for trusted social computing. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas. Each of the Program Areas within the Division balances opportunity-driven research with high risk, high-payoff scientific exploration and needs-driven efforts that look for scientific solutions to the near-term needs of the warfighter.

B. Program Areas

The Computing Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY15, the Division managed research within these four Program Areas: (i) Information Processing and Fusion, (ii) Computational Architectures and Visualization, (iii) Information and Software Assurance, and (iv) Social Informatics. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Information Processing and Fusion. The goal of this Program Area is to understand the fundamental principles and to establish innovative theories for data processing, information extraction, and information integration toward real-time situational awareness and advanced targeting. There are three thrusts for this program area: (i) foundations of image and multimodal data analysis, (ii) data and information fusion, and (iii) active and collaborative sensing. With the ubiquitous availability of data acquisition capabilities in future military operations, effective data and information processing is of increasingly critical importance to defense missions. This program emphasizes mathematical theories, methodologies and algorithms for image understanding, video analysis, and data/information fusion. This research supports the development of novel representations of multimodal data to enable the understanding of multimodal sensor data and contextual information. Also supported is research on detection of events, actions, and activities to extract activity-based intelligence, especially when the events are rare and no extensive training data is available. Potential applications include detection of improvised explosive devices and persistent surveillance.

The increased capability of electronic systems and the proliferation of sensors are generating rapidly increasing quantities of data and information to the point that system operators and commanders are overwhelmed with data and saturated with information. An area of increasing importance is data and information integration or fusion, especially fusion of data from disparate sensors and contextual information. Research activities address several basic issues of data fusion, including information content characterization of sensor data, performance modeling, and the value of information.

2. Computational Architectures and Visualization. The two main Thrusts of this Program Area are Computational Architectures (CA) and Visualization (V). The goal of the CA Thrust is to discover new effective architectures, computational methods, and software tools for future computing systems with special emphasis on the effect that the technological shift to heterogeneous, multi-core processors will have on newly-developed systems. The goal of the V Thrust is to make very large simulations and the visualization of massive data sets more computationally efficient and more interactive for the user. An overarching theme for both Thrusts is the efficient managing and processing of massive data sets. This is due to the fact that the Army's ability to generate data of all types from the battlefield to the laboratory far outpaces the Army's ability to efficiently manage, process, and visualize such massive amounts of information. The CA Thrust attempts to address this issue by investigating innovative architectural designs of both hardware and software components and their interfaces. The V Thrust addresses the issue by investigating innovative algorithms to render massive data sets and/or massive geometric models and to perform large scale simulations of importance to the Army.

The long-term payoffs of the CA Thrust for the Army include new computer modeling and design concepts (or paradigms) as well as software libraries that take advantage of these new multi-core processors and that are scalable (usable on large-scale complex problems and able to handle massive amounts of data) and accurate (precise enough to predict and detect phenomena of interest) for both the laboratory and the battlefield. A payoff associated with the V Thrust is the development of more efficient, interactive, and physically realistic battlefield, training, and scientific simulations.

3. Information and Software Assurance. The goal of this Program Area is to understand the fundamental principles of robust and resilient cyber information systems that can enable the corresponding functions to be sustained under adversarial conditions. The studies guided by this program will enable and lead to the design and establishment of trustworthy computing and communication, regardless of threat conditions. The ARO program on Information Assurance currently has two major Thrust areas: (i) Highly Assured Tactical Information and (ii) Resilient and Robust Information Infrastructure. The goal of the Highly Assured Tactical Information Thrust is to gain new scientific understandings for trustworthy tactical communications and for establishing fundamental principles and to ensure their trustworthiness. The Resilient and Robust Information Infrastructure Thrust promotes research on cyber situation awareness theories and frameworks that combines intrusion prevention, detection, response, and recovery to establish fundamental scientific principles for building mission-sustaining information systems (e.g., software/hardware, computing/communication systems).

Within these research areas, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goal. Research in the Resilient and Robust Information Infrastructure Thrust is focused on exploring and establishing resilient computing and survivability principles, and understanding system trade-offs such as performance, resiliency, and, survivability. The Highly Assured Tactical Information Thrust may lead to the development of novel situation awareness theories and techniques that obtain an accurate view of the available cyber-assets, to automatically assess the damage of attacks, possible next moves, and impact on cyber missions, and also model the behavior of adversaries to predict the threat of future attacks on the success of a mission. The warfighters must have unprecedented situational awareness (including enemy and friendly awareness) at all times. Information assurance must address the delivery of authentic, accurate, secure, reliable, timely information, regardless of threat conditions, over heterogeneous networks consisting of both tactical (mobile, wireless) and fixed (wired) communication infrastructures.

4. Social Informatics. The goal of this Program Area is to quantify technology-based social interaction phenomena, to develop metrics for the quantified phenomena and to develop forensic and predictive analytical and computational models based on these quantifications and metrics. This new Program Area was established in late FY11. The objects of interest will generally be social phenomena (social groups/structure) and socio-cognitive phenomena (human intentions in a social context). The quantification and metrics of interest to this program are those based on domain-scientific principles of social and socio-cognitive science that are at the same time mathematically consistent and computationally feasible. Research of interest to the Program Area includes quantified, analysis-based research about technology-based social interaction phenomena in the following two Thrusts: (i) Quantification and Metrics and (ii) Analytical and Computational Models. Understanding and being able to predict technology-based social networking and social media phenomena will enhance defense in current and future asymmetric conflict, especially in the technology-based component of that defense.

The Quantification and Metrics Thrust focuses on the extraction of information from social media and requires the quantification of and metrics for these phenomena. The metrics by which one measures distance between phenomena will likely be nontraditional. Quantification and metrics need to extend to reliability and accuracy, since falsification and deception are often present at the level of the input into the social medium by a human being. Processing of soft information such as text and voice has been extensively investigated, but insufficiently in the social context that often determines meaning and that can resolve ambiguities.

The Analytical and Computational Models Thrust focuses on analytical and computational models for both forensic and predictive purposes. These models complement the qualitative models of much of sociological research, especially those in the less-investigated area of weak-tie sociology that is important for technology-based social interaction. The models are dependent on the quantification and metrics discussed above as well as on quantitatively expressed social and socio-cognitive principles. Falsification and deception may not be identifiable at the level of input information and may have to be identified by the model. The models should be embedded in applicable sociological and socio-cognitive theory and should not simply be computationally descriptive of social-media phenomena and/or be based only on analogies to physical phenomena.

In 2015, due to reorganization of ARO programs, the Social Informatics program was merged into two other programs: the Social and Cognitive Sciences Program in the Network Sciences Division, and the Social Sciences Program in the Life Sciences Division.

C. Research Investment

The total funds managed by the ARO Computing Sciences Division for FY15 were $19.0 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY15 ARO Core (BH57) program funding allotment for this Division was $4.3 million. The DoD Multidisciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $4.2 million to projects managed by the Division. The Division also managed $5.0 million of Defense Advanced Research Projects Agency (DARPA) programs, $0.6 million of Congressional funds, and $0.4 million was provided by other Army Laboratories. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $0.3 million for contracts. Finally, $4.2 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.1 million of ARO Core (BH57) funds, in addition to any funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY15 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY15 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY15, the Division awarded 20 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Scott Acton, University of Virginia; *Sparse Coding Approach to Spatiotemporal Saliency Detection*
- Professor Pankaj Agarwal, Duke University; *Geometric Graphs for Analyzing Big Spatial Data*
- Professor Ehab Al-Shaer, University of North Carolina - Charlotte; *Agility In Depth: A Formal Framework for Multi-layer Cyber Agility Composition*
- Professor Derek Anderson, Mississippi State University; *Transparent Embedding of Multi-Source Fusion into Pattern Analysis for Handheld Explosive Hazard Detection*
- Professor Richard Baraniuk, William Marsh Rice University; *Information Processing and Fusion via Sparse Factorization*
- Professor John Baras, University of Maryland - College Park; *Noncommutative Probability and Information Theories for Inference from Networked Multi-sensor Data*
- Professor John Cavazos, University of Delaware; *Vulnerability Detection Using Data-flow Graphs and SMT Solvers*
- Professor Kuo-Chu Chang, George Mason University; *Distributed Fusion with Copula*
- Professor Songqing Chen, George Mason University; *Moving Target Defense Through Dynamic Virtual Machine Placement in Clouds*
- Professor Jason Corso, University of Michigan - Ann Arbor; *Action Co-Discovery as a Cross-Reconstruction Problem*
- Professor Gang Hua, Stevens Institute of Technology; *Unified Invariant Representation*
- Professor Robert Kirby, University of Utah; *In Situ Visualization of Discontinuous Galerkin Based High-Order Methods*
- Professor Peng Liu, Pennsylvania State University; *Recognizing Unexplained Behavior in Network Events*
- Professor Hrushikesh Mhaskar, Claremont Graduate University; *Non-stationary Signal Analysis with Applications to Blind-source Processing and Imaging*

- Professor Prasant Mohapatra, University of California - Davis; *Advanced Security Games For Cyber-Physical Systems*
- Professor Ozgur Sinanoglu, New York University; *Investigations into Integrated Circuit Camouflaging*
- Professor Stefano Soatto, University of California - Los Angeles; *Actionable Information-Based Inference for Control and Interaction with Dynamic Scenes*
- Professor Qi Tian, University of Texas at San Antonio; *Scalable Person Re-Identification*
- Professor Yanchao Zhang, Arizona State University; *Sybil-Resilient Influence Measurement in Microblogging Systems*

2. Short Term Innovative Research (STIR) Program. In FY15, the Division awarded five new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor John Benedetto, University of Maryland - College Park; *Super-Resolution and Deterministic Sampling Masks For Image Reconstruction*
- Professor Yan Liu, University of Southern California; *Tensor Completion via Completable Substructure Sampling for Online Spatiotemporal Data Analysis*
- Professor Aswin Sankaranarayanan, Carnegie Mellon University; *Inference in the Compressive Domain*
- Professor Haining Wang, University of Delaware; *Investigation of Pointing Behaviors in Web Browsing*
- Professor Ying Wu, Northwestern University; *Tracking and Identification in Limited Spatial Resolution*
- Professor Stephen Yau, Arizona State University; *An Effective Predictive Approach to Securing Critical Infrastructure through Adaptive Probabilistic Modelling*

3. Young Investigator Program (YIP).

No new starts were initiated in FY15.

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY15 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Institute of Electrical and Electronics Engineers (IEEE) Conference on Communications and Network Security*; San Francisco, CA; 29-31 October 2014
- *Scientific Workshop on Continuously Upgradeable Software Security and Protection*; Scottsdale, AZ; 7 November 2014
- *Vision 2020 and Beyond: Emerging Cyber WarFighting Technologies*; College Park, MD; 10 March 2015
- *IEEE Symposium on Security and Privacy (SP)*; San Jose, CA; 18-20 May 2015
- *8th Association for Computing Machinery (ACM) Conference on Security and Privacy in Wireless and Mobile Networks (WiSec)*; 24-26 June 2015; New York, NY
- *Workshop on Sensing and Analysis of High-Dimensional Data*; Durham, NC; 27-29 July 2015
- *Workshop on Moving Target Defense Quantification,* Fairfax, VA; 31Aug-1 September, 2015

5. Special Programs. In FY15, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded four new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Computing Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. Cyber Situation Awareness. Two MURIs in this topic area began in FY09, with one research team led by Professor Richard Kemmerer at the University of California - Santa Barbara, and the second team led by Professor Peng Liu at Pennsylvania State University. The goal of these projects is to explore cyber situation awareness theories and frameworks. In the long term, this research may ultimately provide more effective defense against cyber attacks, and may lead to new algorithms and systems that can assist human analysts' cognitive situation-awareness processes and decision making.

Complete situation awareness leads to effective defense and response to cyber attacks, especially those launched by adversaries with state sponsorship. The ability to extract critical information and build intelligence leads to a better capability in attack prevention, detection and response and in sustaining critical functions and services. The team is focusing research in the following key areas: (i) situation (knowledge and semantics) representation and modeling that support multi-level abstraction and transformation of data to intelligence, (ii) information fusion that can effectively combine raw and abstracted intelligence of different confidence levels to support optimal response, (iii) uncertainty management and risk mitigation through probabilistic hypotheses/reasoning and sensitivity control, which uses multi-level statistical analysis to manage incomplete and imperfect situation information, (iv) leverage cognitive science understandings to automate human analysts' cognitive situation-awareness processes (to recognize and learn about evolving situations, to create automated hypothesis generation, and to reason in both pre-attack planning and post-attack response), (v) develop a new framework unifying perception, comprehension, and projection functions and integrating situation recognition, impact assessment, trend analysis, causality analysis, and situation response together, (vi) advanced mathematic models for quantitative analysis and assessment of system assurance, and (vii) rapid repair, recovery and regeneration of critical services and functions as part of automatics response to attacks. In this research, novel situation awareness theories and techniques are being investigated to obtain an accurate view of the available cyber-assets and to automatically determine the assets required to carry out each mission task. A proposed situation awareness framework that ties together cyber assets, cyber configuration, attack impact, threat analysis and situation visualization under cyber mission is illustrated in FIGURE 1.

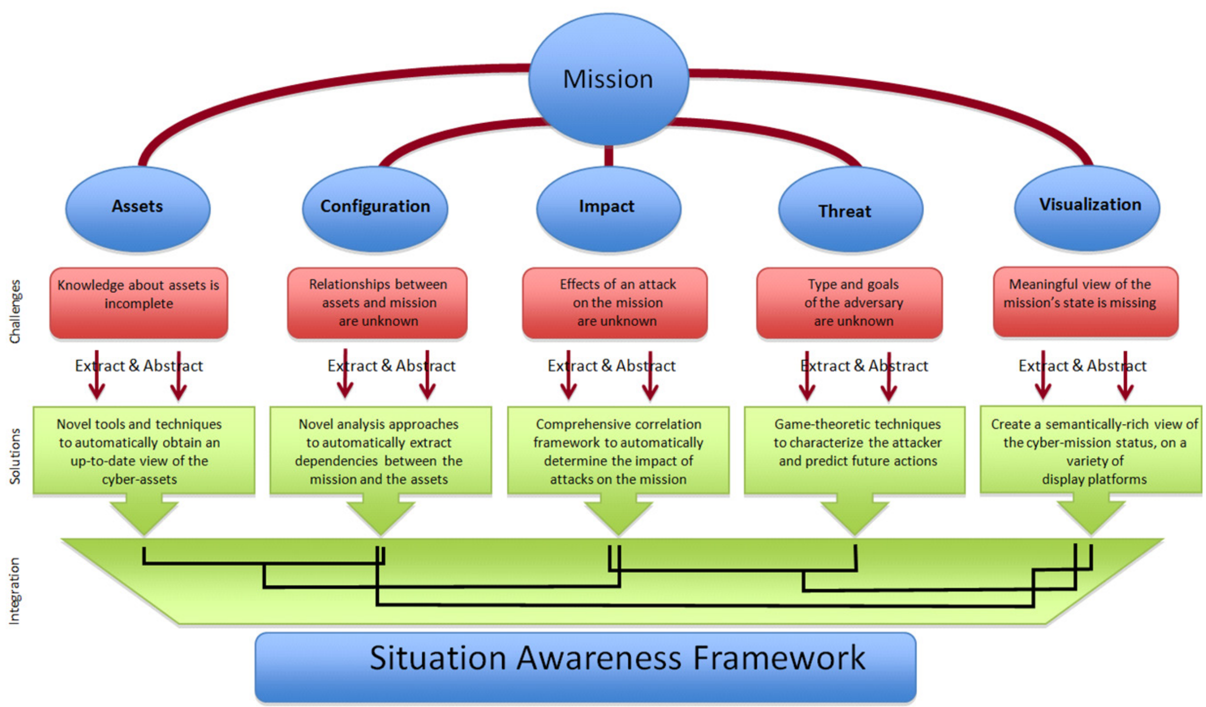

FIGURE 1

Cyber situation framework for attack analysis, prediction, and visualization. This framework incorporates cyber assets, cyber configuration, attack impact, threat analysis, and situation visualization.

2. Principles of Object and Activity Recognition Using Multi-Modal, Multi-Platform Data. This MURI began in FY09 and was awarded to a team led by Professor Richard Baraniuk at Rice University to gain a fundamental understanding of opportunistic sensing and to create a principled theory of opportunistic sensing that provides predictable, optimal performance for a range of different sensing problems through the effective utilization of the available network of resources.

This research includes four focus areas, aimed at developing a theory of sensing that can provide: (i) scalable sensor data representations based on sparsity and low dimensional manifolds that support dimensionality reduction through compressive sensing, (ii) scalable data processing for fusing image data from multiple sensors of potentially different modalities for activity detection, classification, and learning, (iii) opportunistic optimization, feedback, and navigation schemes for multiple mobile sensor platforms that adaptively acquire data from new perspectives to continuously improve sensing performance, and (iv) experimental validation on real-world inputs, such as multi-camera video, infrared, acoustic, and human language.

3. Value-centered Information Theory. This MURI began in FY11 and was awarded to a team led by Professor Alfred Hero III at the University of Michigan. The objective of this MURI is to lay the foundation for a new information theory that applies to general controlled information gathering and inference systems and accounts for the value of information. The theory will be built on a foundation of non-commutative information theory, free probability theory, differential geometric representations of information, and the theory of surrogate information measures. This theory will improve the scientific understanding of the fundamental limits of performance and create better algorithms for extracting and exploiting information in distributed sensor systems.

This research focuses on multiple-modality multiple-sensor fusion problems that use consensus fusion, contextual graphical models, gossip algorithms, and likelihood maps to aggregate information for tracking, surveillance, and other tasks. Topics of interest include resource management in adversarial environments, mobile sensors, and multistage mission planning. Emphasis is placed on creating a powerful theory of actionable information that accounts for value of information and the economic costs of deploying or maneuvering sensors to achieve a particular mission objective. The research comprises three inter-related research themes that collectively address the most critical research challenges in distributed sensing. These thrusts are: (i) information-driven structure learning and representation, (ii) distributed information fusion, and (iii) active information exploitation for resource management. An end-to-end framework will be created that will result in better raw sensor data acquisition and processing, more accurate multi-target tracking, and improved fusion.

4. Adversarial and Uncertain Reasoning for Adaptive Cyber Defense: Building the Scientific Foundation. This MURI began in FY13 and was awarded to a team led by Professor Sushil Jajodia of George Mason University. Adaptive defense mechanisms are essential to protect our nation's critical infrastructure (computing, communication, and control) from sophisticated adversaries who may stealthily observe defense systems and dynamically adapt their attack strategies. This research aims to create a unified scientific foundation to enable the design of adaptive defense mechanisms that will maximize the protection of cyber infrastructure while minimizing the capabilities of adversaries.

The research will leverage recent advances in security modeling, network science, game theory, control theory, software system and network protocol security to create the scientific foundation, which may include general models for defense mechanisms and the systems they protect as well as irrational and rational adversaries. This research will develop a new class of technologies called Adaptive Cyber Defense (ACD) that will force adversaries to continually re-assess, re-engineer and re-launch their cyber attacks. ACD presents adversaries with optimized dynamically-changing attack surfaces and system configurations, thereby significantly increasing the attacker's workloads and decreasing their probabilities of success.

5. Noncommutativity in Interdependent Multimodal Data Analysis. This MURI began in FY15 and was awarded to a team led by Professor Negar Kiyavash at the University of Illinois at Urbana-Champaign. The goal of this research is to establish a new comprehensive information theory for data analysis in noncommutative information structures intrinsic to hierarchical representations, distributed sensing, and adaptive online processing. Methods will be developed based on a novel theory in conjunction with the latest theories of information, random matrices, free probability, optimal transport, and statistical machine learning. They will be applied to the technical domains of causal inference, adaptive learning, computer vision, and heterogeneous sensor networks, and will be validated on real-data test beds including: (i) human action and collective behavior recognition, and (ii) crowd-sourcing in a network of brain-machine interfaces. The framework will provide answers to questions such as: What are the fundamental performance limits for noncommutative information collection and processing systems? What is the effect of side information on noncommutative information structures? How can low complexity proxies for performance be defined that approximate or bound noncommutative performance limits? How can noncommutativity of adaptive measurements be exploited to improve fusion, processing, and planning for distributed sensing systems? When do sequential or partially ordered designs offer significant performance gains relative to randomized designs like compressive sensing?

The approaches for extracting knowledge from complex irreversible partially ordered information structures include but are not limited to introduction of information divergence measures over noncommutative algebras, noncommutative relative entropy measures, and estimation techniques for such measures for high-dimensional data. Accounting for noncommutative structures will result in fundamentally new ways of fusing ordered, directed, or hierarchical organized information in order to support timely decisions at the appropriate level of granularity. Humans learn actively and adaptively, and their judgments about the likelihood of events and dependencies among variables are strongly influenced by the perception of cause and effect, whereas man-made systems only employ correlation-type symmetric measures of dependencies. Research will lead to the development of a theory of decentralized information sharing, causal inference, and active learning inspired by human decision making. Establishment of such a theory for sensing and data processing and application of it to grand challenges in computer vision and brain-computer interfaces will provide new capabilities, including improved time-sensitive, dynamic, multi-source information processing, actuation, and performance prediction guarantees.

C. Small Business Innovation Research (SBIR) – New Starts

Research within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY15, the Division managed one new-start SBIR contract, in addition to active projects continuing from prior years. The new-start project consisted of one Phase II contract. This new-start contract aims to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY15 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY15, the Division managed one new-start STTR contract, in addition to active projects continuing from prior years. The new-start project consisted of one Phase I contract. This new-start contract aims to bridge fundamental discoveries with potential applications. A list of STTR topics published in FY15 and a list of prior-year STTR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY15, the Division managed 10 new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The PECASE winners for each year are typically announced by the White House at the end of the calendar year. However, the FY13-FY15 PECASE recipients had not yet been announced by the end of FY15. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY15, the Division managed 10 new DURIP projects, totaling $1.4 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. Joint NSA/ARL-ARO Advanced Computing Initiative

The Advanced Computing Initiative (ACI) is an ongoing NSA/ARL-ARO joint venture on energy efficient computing. Specifically, energy efficiency is now a primary constraint in designing new supercomputers. In order to provide robust performance, future systems will need to be able to dynamically trade off energy efficiency, performance, and reliability. Started in FY13, the ACI program’s objective is to support research for enabling these tradeoffs and will run for four years at approximately $4 million/year. ARO is responsible for the program management and contracting duties. The ACI program has a close relationship to ARL's High Performance Computing efforts and they offer potential cost savings and reliability benefits for the Army. The costs associated with consuming megawatts of electricity both directly and for the elaborate cooling systems to deal with the excessive heat supercomputers generate are becoming excessive. More important is the machine's reliability as more power to the system means more heat to the components, significantly increasing failure rates. Developing hardware and software infrastructure to increase performance while ignoring the effects on power consumption and reliability will not be feasible in the future. Seven grants have been awarded under the ACI program to teams composed of members from academia, industry and the national laboratories.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Computing Sciences Division.

A. Energy-Efficient, High-Performance, and Reliable Computing

Professor S. J. Ben Yoo, University of California - Davis, Single Investigator Award

The goal of this research is to study, architect, simulate and evaluate the performance of a novel large-scale energy-efficient, high-performance, and reliable computing system based on a new generation of reconfigurable and optically interconnected arrays of many-core systems. To achieve this goal, the UC Davis research team is combining two of their recent innovations. The first is the Asynchronous Array of Simple Processors (AsAP) which is an extremely compact, energy-efficient, fine-grain many-core processor array that has been shown to result in a programmable processing system that sets new levels of performance and efficiency for the computation of a variety of workloads, especially those with computationally-intensive kernels (see FIGURE 2). The second key innovation is the Low latency Interconnect Optical Network Switch (LIONS) that is focused on high energy efficiency with low latency and high throughput exploiting silicon photonics arrayed waveguide grating routers (AWGRs). The combined system based on LIONS and AsAP can scale to support high-concurrency, high-throughput, and low-energy consumption.

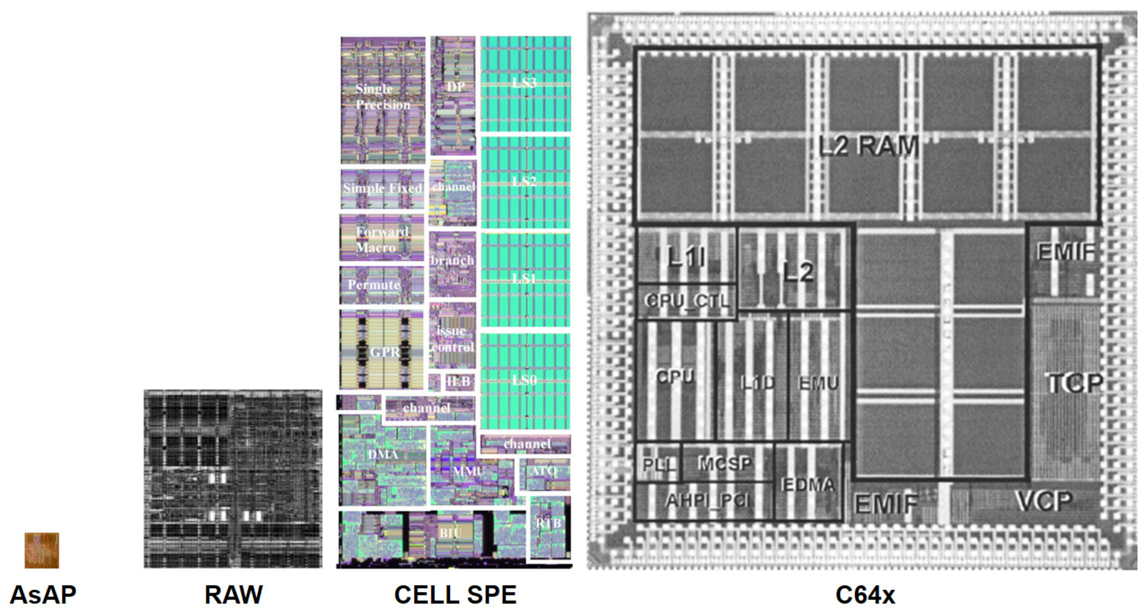

FIGURE 2

Size comparison of AsAP chip to other existing processors. From left to right: UC Davis' AsAP, MIT's RAW, Sony's CELL SPE, and Texas Instruments' C64x.

In FY15, the research team designed, manufactured, and tested a new AsAP chip they named "Kilocore." This new processor array is so named due to the fact that it contains 1024 processors, the first of its kind, i.e., a processor array with over 1,000 working and programmable processors. Other salient features of the chip are: (i) it contains 3072 clock oscillators with each processor being clocked independently of the other processors using a globally asynchronous locally synchronous (GALS) method, (ii) the processor tiles virtually abut (only a few micrometers of inter-processor interconnect), (iii) each core features a network-on-chip (NoC) router with a maximum clock frequency estimated at 2.0 GHz, (iv) each core has two first-in-first-out (FIFO) communication buffers for inter-processor communication that are 64x16-bits each, (v) the instruction memory is 128x40-bits and the data memory is 256x16-bits for each core, and (vi) there are no high-speed global signals implying tremendous scalability. More significantly, this chip has been successfully programmed using a simple data movement scheme where data was successfully transferred from the Kilocore chip to an FPGA and then to a workstation. Although there is still work to be done before Kilocore could be reliably incorporated into high performance computing systems, the UC Davis team's accomplishments to date are significant due to the complexity issues involved in both the manufacturing and programming aspects as well as the potential benefits.

B. Semantic Descriptions of Multi-Object Tracking

Professor Alexander Hauptmann, Carnegie Mellon University, Single Investigator Award

The goal of this research is focused on generating reliable, semantically meaningful descriptions and creating summaries of key aspects of video data given inaccurate/noisy results from the component detectors. With the explosive growth of surveillance video data, automatic summarization of surveillance videos with identity aware visual diaries is an important but unaddressed problem. A visual diary consists of a series of textual descriptions with snapshots that summarize the activities of a person observed in long-term surveillance videos. As a diary is generated for each person, person-specific long-term activity statistics can also be obtained. Identities in visual diaries are critical in many applications such as assessing the health status of nursing home residents. Unlike existing methods that train activity detectors using low-level features for surveillance event detection, this research focuses on generating a summary by tracking framework to automatically generate visual diaries.

In FY15, Professor Hauptmann and his team developed a semi-supervised method for categorizing human actions using multiple visual features. The algorithm simultaneously learns multiple features from a small number of labeled videos, and automatically utilizes data distributions between labeled and unlabeled data to boost the recognition performance. Shared structural analysis is applied in this approach to discover a common subspace shared by each type of feature. In the subspace, the algorithm can characterize more discriminative information of each feature type. This algorithm is robust for action recognition with limited labeled training data.

Much existing research has focused on lab-collected datasets. Considering that labeled real-world videos are difficult to obtain, the team developed an approach to "borrow" strength from existing lab datasets. Though the two data domains are quite different, both characterize human actions. Consequently, it is reasonable to assume that they share components. Therefore, the team designed a solution based on a multi-task learning model to jointly optimize the classifiers for both lab data and real-world data. The general Schatten p-norm is applied on the two classifiers to explore the shared knowledge between them. In this way, the framework is able to mine the shared knowledge between two datasets (see FIGURE 3). This method is easy to implement and an efficient way was proposed to optimize the objective function.

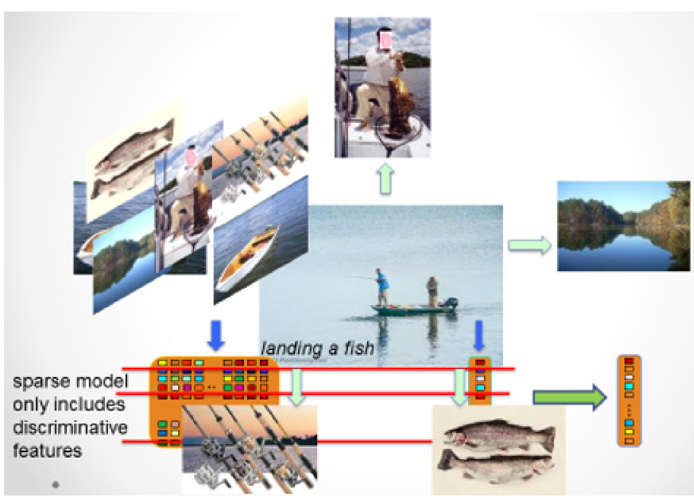

FIGURE 3

High-level semantic analysis. This research provided a framework for high-level semantic analysis with few training examples.

C. Framework of Cyber Deception and Disclosure

Professor Venkatramanan Subrahmanian, University of Maryland - College Park, Single Investigator Award

The goal of this research is to study the interactions between attackers and defenders and establish defensive strategies through the use of deception and selected information disclosure. The research focuses on developing methods to: (i) better understand the adversary and the victim in cybersecurity attacks, (ii) determine a suite of deceptive and disclosed strategies that may enable us to deceive an adversary, and (iii) develop ways of using these strategies to maximize the level of protection afforded to our enterprise.

In FY15, Professor Subrahmanian and his team developed the concept of a system vulnerability dependency graph (SVDG) that can be used to map the vulnerabilities within the enterprise and to understand how the attacker may exploit one vulnerability after another in order to compromise different nodes on the network. The team also created an algebra of operations to manipulate these graphs. Based on the system vulnerability dependency graph, the team established defense strategies which include: (i) deceive the adversary by adding new "honey" nodes to the network, (ii) deceive the adversary by adding new "honey" vulnerabilities to the network, (iii) better protect the network by deactivating some software, and (iv) better protect the network by patching existing vulnerabilities. The derived Pareto-Optimal Defender model suggests that the defender must minimize the maximal expected damage that the adversary can do, while simultaneously minimizing a number of other factors (minimize cost of defending, minimize loss to productivity if some products are deactivated, etc.). FIGURE 4 shows the overall framework that integrates both deception and vulnerability analysis to better defend enterprise networks.

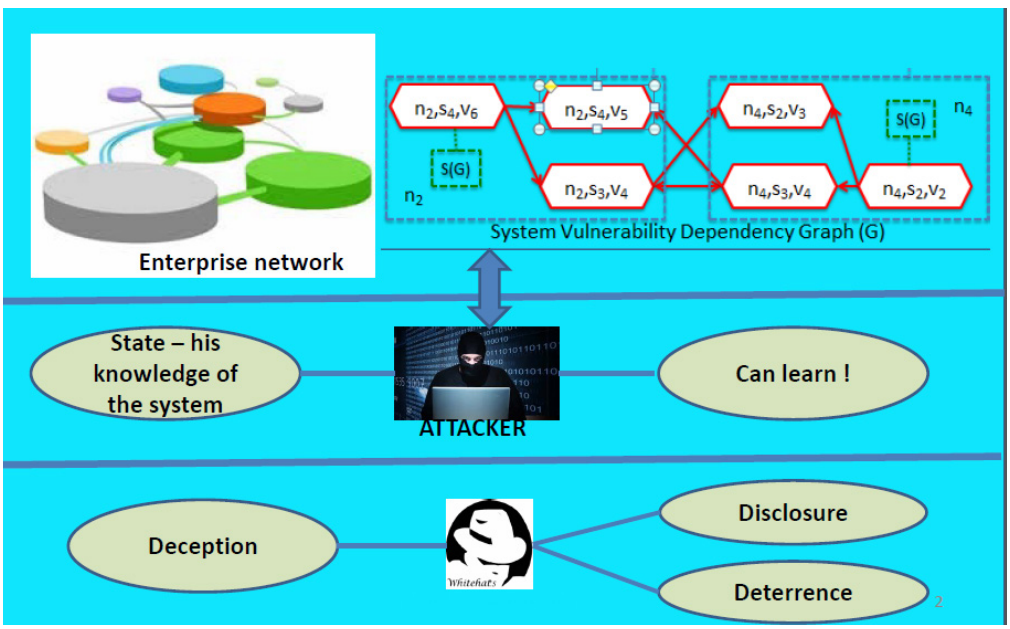

FIGURE 4

Map of a comprehensive cyber defense framework that integrates vulnerability analysis and active defense based on deceptive techniques and selective disclosure.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Approach of Data-Adaptive Union-of-Subspaces to Processing of Imaging Data

Investigator: Professor Waheed Bajwa, Rutgers University, Young Investigator Program Award
Recipient: ARL Sensors and Electron Devices Directorate (ARL-SEDD)

One prominent feature of the current information age is the availability of ubiquitous sensing capabilities that constantly collect various types of data to the degree that analysis and understanding of big data becomes a major challenge facing society. The objective of this research is to establish a new geometric approach to effective data analysis and understanding by exploiting recent advances in the increasingly converging fields of approximation theory, mathematical signal processing, and high-dimensional statistics.

In FY15, Professor Wajwa and his team established two new nonlinear geometric models for data describing "related" objects/phenomena. The first of these models, suited for mildly nonlinear data, is termed the metric-constrained union-of-subspaces (MC-UoS) model, which straddles the two extremes of the subspace model and the union-of-subspaces model. The second one of the models, suited for highly nonlinear data, is termed the metric-constrained kernel union-of-subspaces (MC-KUoS) model, which generalizes the kernel subspace model. Algorithms were designed to efficiently learn a MC-UoS or a MC-KUoS underlying data of interest, and extended to the case when parts of the data are missing. Numerical experiments using both synthetic and real imaging data have demonstrated the superiority of the new geometric models and learning algorithms over existing approaches in the literature.

In addition, the team investigated data-adaptive representations for big, distributed data. The setup in these assumes that a number of geographically-distributed, interconnected sites have massive local data and they are interested in collaboratively learning a low-dimensional geometric structure underlying these data. A novel distributed algorithm, called cloud K-SVD, was created for collaborative learning of a UoS structure underlying distributed data of interest. The goal of cloud K-SVD is to learn an over-complete dictionary at each individual site such that every sample in the distributed data can be represented through a small number of atoms of any one of the learned dictionaries. Cloud K-SVD accomplishes this goal without requiring communication of individual data samples between different sites.

The Aviation and Missile Research Development and Engineering Center (AMRDEC) and ARL-SEDD have met separately with Professor Bajwa to discuss this new approach. The software and algorithms developed as part of this research have been transferred to ARL-SEDD for testing on real-world imaging and video data.

B. Optimal Scheduling of Cybersecurity Analysts for Minimizing Risk

Investigator: Professor Sushil Jajodia, George Mason University, MURI Award
Recipient: ARL Computing and Information Sciences Directorate (ARL-CISD)

Cybersecurity threats are on the rapid rise with evermore digitization of the information that many day-to-day systems depend upon. Current cyber defense systems involve a two step process: (i) anomaly analysis and intrusion detection sensors continuously analyze incoming traffic and data and generate alerts when certain monitoring rules are violated, and (ii) human analysts examine these alerts, build an overall cyber situation picture, and determine the actions to take to mitigate cyber risks. Unfortunately the number of alerts generated is astounding due to the ever increasing volume of data that the system has to analyze while only a portion of these alerts is considered to be significant enough to require thorough examinations by a cybersecurity analyst. Nevertheless, cyber analysts are in short supply today. They have always been overwhelmed by the alert volume, leading to increased cyber risk if not all significant alerts can be examined properly. In addition with analysts possessing different sets of skills and varying levels of expertise, scheduling analyst coverage to minimize cyber exposure risks have been a critical need.

In FY15, Prof. Jajodia developed a generalized optimization model for scheduling cybersecurity analysts to minimize risk (maximize significant alert coverage by analysts) and maintain risk under a pre-determined upper bound. The team tested the optimization model and its scalability on a set of given sensors with varying analyst experiences, alert generation rates, system constraints, and system requirements. Results indicate that the optimization model is scalable, and is capable of identifying both the right mix of analyst expertise in an organization and the sensor-to-analyst allocation in order to maintain risk below a given upper bound. Several meta-principles were derived from the optimization model which serve as guiding principles for hiring and scheduling cybersecurity analysts (see FIGURE 5). This new approach has been transitioned to ARL-CISD with a joint patent disclosure and an optimal scheduler is being tested at ARL-CISD.

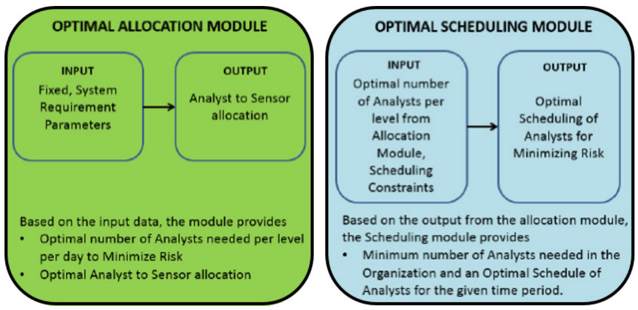

FIGURE 5

Cybersecurity analyst optimal allocation and scheduling framework to minimize risk.

C. Adaptive Scheduling for High Performance Computing

Investigators: Professors V. Sarkar, D. Sbirlea, and Z. Budimlic, Rice University, Single Investigator Award
Recipient: Intel Corporation

The goal of this research is to design and integrate new runtime software with leading-edge hardware to deliver novel capabilities for monitoring and control and for interfacing with the programming environment in order to balance computational performance with energy efficiency. The approach adopted in this research assumes a 3-dimensional space with axes representing energy, performance, and resilience, and choices for computational tasks (EDTs) and data blocks to be placed in this space (see FIGURE 6). The amount of interaction between the axes depends on both the application and the particular machine in question. Past work on OS-level adaptive scheduling and heterogeneous processor scheduling has shown the benefits of adaptive runtime optimization for performance. The challenges for this approach include adding energy efficiency and reliability dimensions to the optimization space, while simultaneously considering both computation and data placement.

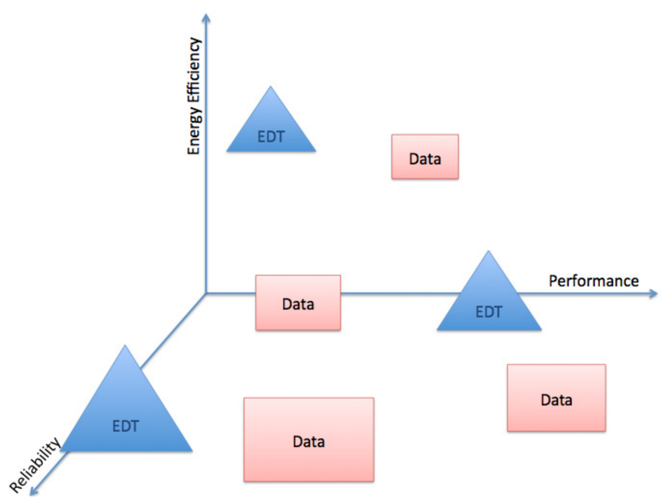

FIGURE 6

Notational 3-dimensional graph depicting the placement of tasks and data to optimize dynamic tradeoffs among performance, energy efficiency, and reliability.

In FY15, this team of researchers has teamed up with computer scientists from Intel and designed extensions to runtime systems that enable adaptive scheduling with different task granularities and different numbers of active workers. For automatic selection of task granularity, they extended their Advanced Computing Runtime (ACR) system to adapt to different chunk sizes per workers, and different numbers of workers. The adaptation to different chunk sizes per workers is also applicable to cores with non-uniform clock frequencies. For different numbers of workers, they demonstrated how their ACR system can dynamically select the number of workers to minimize the energy-delay product by minimizing throughput per workers for benchmarks such as UTS (Unbalanced Tree Search). These scheduling extensions have been incorporated into Intel's Open Community Runtime (OCR) framework.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, some ARO-funded research efforts are on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Hybrid Spectrum Face Detection and Recognition: Theory and Algorithms

Professor Jingyi Yu, University of Delaware, Single Investigator Award

This research focuses on creating a new collaborative, multi-spectrum sensing framework for face detection and recognition under low lighting conditions. By leveraging computational multi-spectrum imaging and multimodal image analysis, solutions based on the new framework will be able to robustly track, detect, and recognize single or multiple target faces under poor lighting conditions such as in complete darkness. A new class of feature extraction methods based on various properties of the face and skin will be established to isolate and extract desired data. The new features will exploit the latest advances on skin color segmentation, principal component analysis, eigen-space modeling, histogram analysis, texture analysis, and discriminatively-trained scanning window classifiers. The new features will be validated under the Viola-Jones detector for effectiveness. With those features, a new 2.5D multi-spectrum face recognition algorithm will be designed.

In FY16, it is anticipated that a 3D deformable model will be built to conduct fast 3D model fitting. The algorithm uses eye location and coarse depth information to fit the canonical face model to the acquired 2.5D data for estimating the face pose. The eye locations will be used as the landmarks (hard constraints) when conducting shape fitting through non-linear optimization. Once the 3D model is obtained, 3D face recognition algorithms can then be applied.

B. Vulnerability Detection

Professor John Cavazos, University of Delaware, Single Investigator Award

The goal of this research is to create algorithms and methods that will allow users to quickly detect vulnerabilities in an executable using an SMT (Satisfiability Modulo Theory) solver, without the need to access the source code of the application. Current vulnerability detection techniques require source code of the application to be analyzed. It is often the case in the real world that one does not have access to the source code. For example, the application being analyzed could be a third-party application or the source code could simply not be available. Thus, being able to statically analyze an executable (i.e., a binary) would be extremely advantageous. However, analyzing a binary is hard and time consuming. In order to overcome the difficulties associated with analyzing binaries, the ROSE Compiler will be utilized, which has been used successfully in the past for decompilation. The ROSE Compiler has the ability to generate data flow graphs that can then be analyzed for various vulnerabilities. The next step would be to explore different methods of phrasing the problem of vulnerability detection in binaries as an SMT problem and then adapt and/or enhance an existing SMT solver to address the potentially large state space due to the extremely large data flow graphs expected to be generated by this process.

In FY16, efficient algorithms will be developed that allow users to quickly detect vulnerabilities in executables using an SMT solver, without the need for access or availability to the source code of the application. If successful, such methods will allow the Army, in general, and the Communications-Electronics Research, Development and Engineering Center (CERDEC) in particular, to analyze many millions of lines of assembly code from binaries, thus reducing the time and the kinds of expertise necessary to detect vulnerabilities in any application of interest.

C. A Formal Framework for Multi-layer Cyber Agility Composition
Professor Ehab Al-share, University of North Carolina - Charlotte, Single Investigator Award

The goal of this research is to address the fundamental challenges of forming a systematic composition of various agility techniques in a single framework that can increase the overall agility effectiveness nonlinearly while assuring the integrity, security and performance properties of the system. Novel and transformative approaches to formulate a prescriptive framework called Agility-in-Depth will be investigated to instantiate a new composite agility strategy that is (i) correct-by construction, (ii) resilient against adaptive adversaries, and (iii) capable of exploiting the complementary and overlapping capabilities among different agility mechanisms.

In FY16, the PI will establish an Agility-in-Depth framework that can provide (i) efficiency: the defense effectiveness of the composite agility is much greater than the sum of the individual ones (e.g., increasing uncertainty, defending multiple attacks); (ii) cost-effectiveness: the overhead cost of the composite agility is linearly comparable to the sum of individual costs; and (iii) safety: satisfies the system requirements and maintains the global consistency among different agility mechanisms. The results of this research will enable new theoretical foundations and transformative approaches in the science of cyber agility by contributing to the understanding of automated reasoning for cyber agility composition and synthesis.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Cliff Wang
Division Chief
Program Manager, Information and Software Assurance

Dr. Mike Coyle
Program Manager, Computational Architectures and Visualization

Dr. Liyi Dai
Program Manager, Information Processing and Fusion

B. Directorate Scientists

Dr. Randy Zachery
Director, Information Sciences Directorate

Dr. Bruce West
Senior Scientist, Information Sciences Directorate

Ms. Anna Mandulak
Contract Support

C. Administrative Staff

Ms. Debra Brown
Directorate Secretary

Ms. Diana Pescod
Administrative Support Assistant

CHAPTER 5: ELECTRONICS DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2015* is to provide information on the programs and basic research supported by ARO in fiscal year 2015 (FY15), and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Electronics Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY15.

A. Scientific Objectives

1. Fundamental Research Goals. The principal objective of research in the ARO Electronics Division is to discover phenomena that involve elementary particles and wave phenomena in solid state materials and plasma. More specifically, the Division supports basic research to discover and control the relationship between nanostructure and heterostructure designs and charge transport and carrier recombination dynamics, to understand and improve the stimulus-response properties of electronic materials/structures, to leverage nanotechnology for enhanced electronic properties, to comprehend and mitigate distortion and noise, to understand and exploit complex electromagnetic and acoustic structures and propagation, and to explore ultra-fast, solid state and plasma mechanisms and concepts. The results of this research will stimulate future studies and help keep the U.S. at the forefront of research in electronics by revealing new pathways for the design and fabrication of novel electronic structures that have properties that cannot be realized with current technology.

2. Potential Applications. Electronics research is relevant to nearly all Army systems; therefore, research under this program provides the underlying science for a wide variety of developmental efforts and contributes to the solution of technology-related problems throughout the full spectrum of the Army's "System of Systems." Army-relevant research in electronics spans areas such as (i) nano- and bio-electronics to provide components that require less power, interface with biological systems, and enhance the creation and processing of information, (ii) studies in electromagnetics, acoustics, microwaves, and power to enable multimodal sensing for detection, identification, and discrimination of environmental elements critical to decision-makers in complex, dynamic areas , including defeat of electronic threat systems, (iii) optoelectronics, which involves the creation and use of electromagnetic radiation from far infrared to X-ray for sensing, communication and to interrogate, disrupt, and defeat hostile infrared sensor systems and (iv) action-reaction relationships in electronic materials and structures that may lead to new devices and methods for sensing and communication over long ranges and within complex environments.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Electronics Division coordinates and leverages research within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the Defense Advanced Research Projects Agency (DARPA), as well as the various DOD Labs and other governmental activities with electronics research missions. Moreover, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, sensing is a research element of all ARO Divisions, and the Electronics Division serves as the focal point for ARO sensing research. Specific interactions include joint projects with the Physics Division that promote research for physics-based understanding of semiconductor materials, non-reciprocal materials and devices, propagation effects, plasma devices, and stimulus response effects in condensed matter. The Electronics Division also coordinates its research portfolio with the Materials Science Division to pursue the design and characterization of new materials and structures, the evaluation of electrical properties, and the study of electronic processes at the molecular level. This Division complements its research initiatives in the Chemical Sciences Division to include research to understand how chemical changes and chemical structures influence electrical, magnetic, and optical properties and investigations of high frequency spectroscopic techniques for use in chemical defense, especially explosive detection. The Life Sciences Division's Program Areas also interface with electronics research in areas of biological detection as well as interfacing to biological organisms. Lastly, creating computational methods and models for target recognition and understanding nano-molecular structures and carrier transport shared research goals between the Electronics and Information Sciences Divisions.

B. Program Areas

The Electronics Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY15, the Division managed research within four Program Areas: (i) Nano- and Bio-electronics, (ii) Electromagnetics and Radio Frequency Electronics, (iii) Optoelectronics, and (iv) Electronic Sensing. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have long-term objectives that collectively support the Division's overall objectives.

1. Nano- and Bio-electronics. The program will involve the creation of novel electronic devices including nano- and bio-based sensors and transducers based on semiconductor electronics and hybrid molecular-semiconductor devices in addition to organic-inorganic hybrid materials. This project supports basic research that will apply biology concepts to electronics and photonics to create biomimetic structures and devices for information processing, information storage, electronic components, and actuators. It will also create unique electronic sensors at the nano to the macro level that interface with biological materials in order to extract information on biological systems. The long term goal of this task is to discover and control novel phenomena by the combination of electronics, photonics, and bioscience to provide novel electronic technological capabilities for defense-related applications such as sensing, data processing, communications, target recognition, navigation, and surveillance.

2. Electromagnetics and Radio Frequency Electronics. This program area is concerned with investigation of electromagnetic (EM) and radio frequency (RF) phenomena for integrated antenna arrays, multifunctional antennas, EM power distribution, and new sensing modalities. It also explores acoustic phenomena and new concepts for circuit integration for greater functionality, smaller size/weight, lower power consumption, enhanced performance, with focus in the frequency regime from low to terahertz frequencies.

This area addresses the science behind new approaches to the generation, transmission, and reception of EM power and signals. Emphasis is placed on the HF through terahertz spectrum, however, novel ideas at lower frequencies down to direct current may be addressed. In the RF regime orders of magnitude improvements in systems performance, cost, weight, reliability, size characteristics, and functionality will be sought. Issues include the coupling of EM radiation into and out of complex structures, antennas, both active and passive, transmission lines and feed networks, power combining techniques, EM wave analyses of electrical components, and EM modeling techniques. Thermal problems stemming from the concentration of higher and higher power into smaller and smaller volumes will be addressed. Antenna research will break away from the methodologies that were developed for continuous-wave, narrowband, steady-state operation to invent new design techniques, architectures, and materials that can dramatically increase the radiation efficiency and bandwidth of tactical antennas while simultaneously reducing their size and signature. The EM and acoustic detection and analysis of underground targets, landmines, and IED's will continue to be of interest. Unusual propagation effects in the atmosphere and gaseous plasmas offer new opportunities for sensing and detection. Army applications of this technology include communications (both tactical and strategic), command and control, reconnaissance, surveillance, target acquisition, and weapons guidance and control.

3. Optoelectronics. The goal of this Program Area is to discover and control novel nanostructure and heterostructure designs for the generation, guidance, and control of optical/infrared signals in both semiconductor and dielectric materials. The research in this program may enable the design and fabrication of new optoelectronic devices that give the Soldier high-data-rate optical networks including free space/integrated data links, improved IR countermeasures, and advanced 3D imaging. This program has three Thrust areas: (i) High Speed Lasers and Interconnects, (ii) Ultraviolet and Visible Photonics, and (iii) Mid-infrared Lasers. The research topics seek to overcome slow spontaneous lifetimes and gain dynamics, low carrier injection efficiency, poor thermal management, and device size mismatches. Novel light emitting structures based on III-V compounds, wide bandgap II-VI materials, rare-earth doped dielectrics, and silicon nanostructures are being investigated along with advanced fabrication and characterization techniques. Nanotechnology is exploited to allow interfacing of optoelectronic devices with electronic processors for full utilization of available bandwidth. Electro-optic components are being studied for use in guided wave data links for interconnections and optoelectronic integration, which are all requirements for high speed full situational awareness. In addition, emitters and architectures for novel display and processing of battlefield imagery are also important.

4. Electronic Sensing. The goal of this Program Area is to extend the underlying science behind action-reaction relationships in electronic materials and structures as well as understand target signatures. This Program Area is divided into two research Thrusts: (i) Photonic Detection and (ii) Thermal, Mechanical, and Magnetic Effects. The scientific objective of Photonic Detection is to understand and control the direct conversion of light to charge in infrared materials and structures. This includes the design and fabrication of novel detector structures, such as superlattice or barrier structures, as well as novel plasmonic effects. An important element in this thrust area is the reduction of performance limiting defects in semiconductor material and structures through lattice matching and other methods. Development of novel characterization techniques is also explored to determine the fundamental issues behind carrier transport, lifetimes, and noise. The Thermal, Mechanical, and Magnetic Effects Thrust includes the modalities of acoustic, magnetic, infrasound, as well as thermal effects for infrared detection. Research in this Program Area seek to give the Soldier 100% situational awareness of vehicles, personnel, weapon platforms, projectiles, explosives, landmines, and improvised explosive devices (IEDs), in day/night, all weather, and cluttered environments through natural and man-made obstructions.

C. Research Investment

The total funds managed by the ARO Electronics Division for FY15 were $28.5 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY15 ARO Core (BH57) program funding allotment for this Division was $5.8 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $5.9 million to projects managed by the Division. The Division also managed $1.3 million of Defense Advanced Research Projects Agency (DARPA) programs, $0.8 million of Congressional funds and $6.7 million provided by other Federal agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $3.3 million for contracts. Finally, $4.7 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.5 million of ARO Core (BH57) funds, in addition to any funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY15 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY15 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY15, the Division awarded 22 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Ehsan Afshari, Cornell University; *Microwave-Enhanced Nanoscale Magnetic Resonance Imaging of Individual Biomacromolecules*
- Professor Arturo Ayon, University of Texas at San Antonio; *Modeling, Fabrication and Characterization of Self-Aligned 2D and 3D Nanowire Arrays for Terahertz Operation*
- Professor Seth Bank, University of Texas at Austin; *Highly-Strained Mid-Infrared Diode Lasers*
- Professor Shannon Blunt, University of Kansas; *Cognitive Radar to Address Spectral Congestion*
- Professor Philip Bos, Kent State University; *Research of Liquid Crystal Properties for Micro-Photonic Devices*
- Professor Russell Dupuis, Georgia Tech Research Corp.; *Fundamental Studies of Growth and Processing of III-N-based deep UV solar-blind back-side-illuminated Separate Absorption and Multiplication*
- Professor Philippe Guyot-Sionnest, University of Chicago; *Electronic Relaxation and Doping in Small Gap Colloidal Quantum Dots*
- Professor Donhee Ham, Harvard University; *CMOS-Enabled Massively-Parallel Intracellular Nanowire Array as a New Neuroscience Tool and its Biotic-Abiotic Hybrid Application for Micro-Neuroprosthesis*
- Professor James Hwang, Lehigh University; *Fundamental Theoretical and Experimental Study of Nanoporation of Biological Cells by Novel Electrical/Optical Detection and Imaging*
- Professor Albena Ivanisevic, North Carolina State University; *Development of Gallium Nitride Based Interfaces*
- Professor Brian LeRoy, University of Arizona; *Creating and Imaging van der Waals Heterostructures*
- Professor Zhenqlang Ma, University of Wisconsin - Madison; *Bio-Hybrid Electronics and Synthetic Neuron Circuits*
- Professor Zetian Mi, McGill University; *Electrically Injected 280 nm AlGaN Nanowire Lasers on Silicon*
- Professor Howard Milchberg, University of Maryland - College Park; *Applications of Femtosecond Filament-Tailored Atmospheric Gas Density Profiles*

- Professor Ram Narayanan, Pennsylvania State University; *Investigation of Nonlinear and Cognitive Radar Approaches for Target Detection*
- Professor Shriram Ramanathan, Harvard University; *Mott Transistor: Fundamental Studies and Device Operation Mechanisms*
- Professor Manijeh Razeghi, Northwestern University Evanston Campus; *A Comprehensive Study of Surface Defects in traditional Type II InAs GaSb Superlattices and Ga free Type II*
- Professor Joseph Talghader, University of Minnesota - Minneapolis; *Photon Statistics and Spectral Selectivity Limits of Thermal Detectors*
- Professor Kang Wang, University of California - Los Angeles; *Interface Physics and Applications in Topological Insulator-based Magnetic Heterostructures*
- Professor Peide Ye, Purdue University; *Ballistic Phosphorene Transistor*
- Professor Zhi-Gang Yu, Washington State University; *Cross-linked Metal Particles for Low-noise Bolometer Materials*
- Professor Lin Zhu, Clemson University; *High Power, Single Frequency, Broad-area Diode Laser Emitters/Arrays and their Applications in Microresonator Based Frequency Combs*

2. Short Term Innovative Research (STIR) Program. In FY15, the Division awarded 13 new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Mikhail Belkin, University of Texas - Austin; *Hybrid Quantum Cascade Lasers on Silicon-on-sapphire*
- Professor Elif Ertekin, University of Illinois - Urbana - Champaign; *Rapid Identification of Optimal Dopants for Silicon Based Broadband Infrared Detectors via Quantum Mechanical Simulation*
- Professor Albena Ivanisevic, North Carolina State University; *Semiconductor Materials for Neuronal Interfaces*
- Professor Jacob Khurgin, Johns Hopkins University; *Mitigating the loss in plasmonics and metamaterials*
- Professor Xiaoqin Li, University of Texas at Austin; *Probing Quasiparticle Transport Using Spatially Resolved Ultrafast Spectroscopy*
- Professor Vinod Menon, CUNY - City College of New York; *Solution Processed ZnO Nanoparticle Based UV Lasers*
- Professor Amir Mortazawi, University of Michigan - Ann Arbor; *An Efficient Near-Field Wireless Power Transmission System*
- Professor Hossein Mosallaei, Northeastern University; *Designer Solids Nanoantennas and Materials*
- Professor Kamal Sarabandi, University of Michigan - Ann Arbor; *Wideband Low-Frequency Antenna Formation Using a Cluster of Near-field Coupled Small Antennas*
- Professor Fatemeh Shahedipour-Sandvik, The Research Foundation of SUNY; *Betavoltaic Device with Enhanced Performance using WBG (Al)GaN Nanostructures*
- Professor Roman Sobolewski, University of Rochester; *Self-Switching Nano-diodes for Generation and Detection of THz Radiation*
- Professor Kang Wang, University of California - Los Angeles; *Magnetic topological insulator enabled spin-orbit torque device application*
- Professor Michael Weimer, Texas A&M University; *Atomically Accurate Structure Analysis for InAs / InAsSb Strained-Layer Superlattice*

3. Young Investigator Program (YIP).

No new starts were initiated in FY15.

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY15 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *31st International Annual Review of Progress in Applied Computational Electromagnetics Conference*; Williamsburg, Virginia; 22-26 March 2015
- *IEEE Wireless Power Transfer Conference*; Boulder, CO, 13-15 May 2015
- *Advanced Research Workshop on Future Trends in Microelectronics*; Mallorca, Spain; 21-26 June 2015
- *70th International Symposium on Molecular Spectroscopy*; Champaign-Urbana, IL; 22-26 June 2015
- *Workshop Emergent Nontrivial Phenomena in Quantum Heterostructures and Their Applications in Electronics*; Los Angeles, CA; 11-12 August 2015

5. Special Programs. In FY15, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded seven new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Electronics Division; therefore, all of the Division's active MURIs are described in this section.

1. Near and Far-Field Interfaces to DNA-Guided Nanostructures from RF to Lightwave. This MURI began in FY10 and was granted to a team led by Professor Peter Burke at the University of California - Irvine. The goal of this research is to develop new sensing modalities for chem/bio sensing based on materials development in nanotechnology and nanoscience, and to interface nano-electronic and nano-optical components to biologically relevant physical properties.

In order to tap the requisite contributions from different academic disciplines (DNA chemistry, electrophysiology, nano-electronics, optics and THz spectroscopy), three sensing hardware testbeds are being developed for further testing, functionalization, and analysis: (i) bottom up carbon electronics (graphene, nanotubes); (ii) top down silicon nano-electronics (top down Si nanowires); and (iii) nano-optics (CdSe and other nanowire emitter/detector architectures). Two functionalization schemes are being be applied to these testbeds to enable sensing: DNA origami aligned to nanowire arrays and ion channel functionalization for electrophysiology at the nanoscale. Unique aspects of this sensing research include multiplexing (massively parallel sensor arrays) via DNA self-assembly. Using this approach, in principle, each nanowire in an array can have a different sensing functionality, at unprecedented pitch. In addition, direct integration of bio-electrical signals (ion channel currents) to nano-electrodes (carbon, silicon, and nano-optics) are being explored. A key discovery in the recent year is that the ion channel current pulses can be used to charge the quantum capacitance of graphene, demonstrating a qualitatively new sensing modality for nanoscale electrophysiology. Lastly, single-molecule sensitivity and novel mechanisms for selectivity at THz frequencies are being pursued. Once the three test beds are functionalized, their THz spectra may provide non-trivial information about chemical composition. Advances in this MURI will enable a new class of sensors for applications in biomedical diagnostics for civilian and warfighter health care, chemical agent detection, nano-optical devices for sensing, and neural-electrical interface at unprecedented spatial resolution.

2. Defect Reduction in Superlattice Materials. This MURI began in FY11 and is led by Professor Daniel Wasserman at the University of Illinois - Urbana Champaign. The team consists of researchers from Arizona State University, Georgia Tech, and the University of North Carolina - Charlotte. The objective of this project is to determine and understand the relationship between minority-carrier lifetimes and classes of defects in superlattice materials and to formulate strategies for growth and post processing to eliminate or mitigate defects.

This research effort includes an in-depth study of the origins and structural, electrical and optical properties of defects, in-situ and ex-situ probing of defects during growth and fabrication, an investigation of defect reduction techniques, a study on ways to minimize the impact of defects on performance, and testing of results through fabrication and characterization of superlattice structures and devices. Understanding defects at the basic level in these superlattice materials will promote advancements in lasers and modulators as well as infrared detectors. For detectors, lifetime improvements will allow the next generation of focal plane arrays with increased long wave resolution, much larger array formats, broader spectral range into the very long wave infrared, and higher operating temperature to reduce life cycle costs.

C. Small Business Innovation Research (SBIR) – New Starts

Research within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY15, the Division managed six new-start SBIR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of five Phase I contracts and one Phase II contract. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY15 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY15, the Division managed eight new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of seven Phase I contracts and one Phase II contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of STTR topics published in FY15 and a list of prior-year STTR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY15, the Division managed four new ARO (Core) HBCU/MI projects and six new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE)—New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The PECASE winners for each year are typically announced by the White House at the end of the calendar year. However, the FY13-FY15 PECASE recipients had not yet been announced by the end of FY15. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY15, the Division managed seven new DURIP projects, totaling $1.2 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. JTO Multidisciplinary Research Initiative (MRI) Programs in High Energy Lasers

ARO currently manages nine MRI programs for the High Energy Laser Joint Technology Office (HEL-JTO) in Albuquerque (managed by OSD). Six of those are 2012 start MRIs and three of those were awarded through ARO's Electronics Division (the others through Materials and Physics). The three 2010 start MRIs are led by professors at the University of New Mexico, the University of Central Florida (Center for Research in Electro-Optics and Lasers), and Clemson University. These three MRIs were reviewed in FY15 and 2 of the three are ending this year. The Clemson all-solid photonic bandgap fiber laser MRI has been selected for a continuation effort of 2 additional years. The foci of the other two ending MRIs were: optical techniques for characterizing high power handling optical coatings and methods for improving their reliability, uses and fundamental material loss improvement and beam combining techniques with volume Bragg gratings. The 2012 start MRIs are led by professors at Rutgers, University of Illinois, Texas Tech, University of California – Riverside, Clemson, and the University of Central Florida (Center for Research in Electro-Optics and Lasers). These MRIs are on the following topics: single crystal fiber lasers, reduced stimulated Brillouin scattering fiber materials, rare-earth doped GaN, polycrystalline AlN ceramic gain media, leaky wave and gas-filled hollow-core fiber lasers, and nonlinearity mitigation in fiber lasers. The 2012 start MRIs were reviewed this year for the option year funding decisions and all of them were selected to continue. ARO continues to play a significant role in leading the MRI programs by organizing kickoff meetings and program reviews, particularly in conjunction with the HEL-JTO Advanced Concepts Technical Area Working Group which leads the more basic research endeavors that HEL-JTO supports. The ARL Computational and Information Sciences Directorate (ARL-CISD) and the ARL Sensors and Electron Devices Directorate (ARL-SEDD) participate in HEL-JTO program evaluation through annual reviews.

I. DARPA High Power Efficient and Reliable Lasers (HiPER) I Program

The objective of this program is to develop compact, efficient and bright laser-diode (LD) sources that will result in extremely light-weight and inexpensive high-energy lasers (HELs) for the U.S. military. The SRL technologies developed in the HiPER I program will increase the power-to-weight ratio of LD pumps for HELs. This program follows on the previous DARPA/ARO funded program, HiPER I. HiPER II takes the thermal modeling efforts of HiPER I and pushes the entire pump module forward to create an array of modules that will be used in the DARPA EXCALIBUR. ARO is involved in this program by providing assistance in leveraging technical knowledge of many related JTO-HEL programs and DARPA's EXCALIBUR phased array program. ARL-CISD phased array group has helped transition its technology into the EXCALIBUR program, which uses fiber lasers to achieve beam steerable laser arrays. Integrated diode laser bars may provide further miniaturization to such systems. The work on this program ended in FY15, and the results showed potential for even further improvements in laser bar efficiency for both wall-plug efficiency and coupling efficiency.

J. DARPA High Power Laser Diode Facet Passivation Program

Another follow-on program to HiPER II is a result of discoveries that catastrophic optical mirror damage (or COMD) continues to plague laser bar power limits. ARO led discussions with Science Research Lab (SRL) which led to this ARO/DARPA effort as well as an ARO/DARPA SBIR. DARPA and ARO began a program to systematically study and understand the optimal facet passivation. ZnSe is known to be used in a number of laser diode commercial products, but other opportunities exist for better lattice matching and thermal expansion matching. Much of the effort is focused on using materials similar to those used in the laser itself. DoD will benefit from these studies as they help identify the best materials and processes to complete the passivation, which may lead to further improvements in power handling. Progress in the past year has been made in learning to grow the passivation materials epitaxially with further work forthcoming to characterize their performance.

K. DARPA Advanced Wide FOV Architectures for Image Reconstruction and Exploitation (AWARE)

The AWARE program focuses on technologies to enable wide FOV, higher resolution and multi-band imaging for increased target discrimination and search in all-weather day/night conditions. The Electronics Division coordinates research with this program by identifying and monitoring basic research projects with complementary goals. In FY15, the AWARE program provided continued funding for a university project that is based on a result from the Electronics Division's single investigator program.. The objective is to create a three-dimensional imaging platform that allows the field of view of 4 pi Steradian, i.e., a completely spherical imager.

L. DARPA Low Cost Thermal Imaging – Manufacturing (LCTI-M)

The Low Cost Thermal Imager - Manufacturing (LCTI-M) program seeks to enable widespread use of infrared imaging technology by individual warfighters and insertion in small systems. The Electronics Division coordinates research with this program by identifying and monitoring basic research projects with complementary goals. In FY14, the LCTI-M program provided funding for an ongoing project to create free standing bolometer structures with thinner layers, lower heat capacity, and improved imaging performance over existing structures by use of atomic layer deposition. This was a joint project with the University of Colorado and DRS Technologies. ARO is the technical monitor for this project because of a previous association with an ARO MURI concerning uncooled materials.

M. DARPA Efficient Linearized All-Silicon Transmitters ICs (ELASTx) Program

The goal of the ELASTx program is to enable monolithic, ultra-high power efficiency, ultra-high linearity, millimeter-wave, silicon-based transmitter integrated circuits (ICs) for next-generation military microsystems in areas such as radar and communications. The ARO Electronics Division currently co-manages two university grants within this program that are exploring quasi-optical power combining of Doherty amplifiers, and asymmetric multilevel outphasing of large numbers of transistor amplifiers. The program will lead to revolutionary increases in power amplification efficiency while simultaneously achieving high linearity for digitally modulated signals. Prototype ELASTx amplifiers are being tested by scientists in ARL-SEDD for potential use in Army radar and communications systems.

N. DARPA Microscale Plasma Device (MPD) Program

The goal of the MPD program is to support fundamental research in the area of microplasma device technologies and substrates for operation in extreme DoD-relevant environments. The ARO Electronics Division currently co-manages two grants within this program that will develop fundamentally new fast-switching microplasma devices, develop modeling and simulation design tools, and demonstrate the generation of a plasma with an extremely high charge density (1020 - 1022 unbound electrons per cubic centimeter) in a sealed cell with solid walls. This charge density is four to six orders of magnitude larger than is achieved in current microplasma research and is comparable to the carrier density in metallic materials. Research results will be communicated to ARL-SEDD Electronics Technology Branch scientists in order to identify opportunities for technology transfer. If successful, the MPD program will provide proof-of-concept for fast-switching microplasma devices that may enable new sources of radiated energy at sub-millimeter wave and terahertz frequencies, the enabling science behind new high resolution imaging radar and covert communication systems.

O. DARPA High Frequency Integrated Vacuum Electronics (HiFIVE) and THZ Electronics Programs

The long-term vision for the DARPA THZ Electronics program is to develop the critical device and integration technologies necessary to realize compact, high-performance electronic circuits that operate at center frequencies exceeding 1012 cycles per second (i.e., 1 THz). The DARPA HiFIVE program will develop a compact, efficient source of electromagnetic energy capable of generating 100 W with 5 GHz bandwidth at 220 GHz using innovative cold cathode and micromachining technologies. The ARO Electronics Division and ARL-SEDD Electronics Technology Branch co-manage projects within these programs with a goal of using silicon micromachining and MEMS processes to produce precision interaction structures scaled for these extremely small wavelengths. These programs have a high potential impact on military communications, ECM, and radar systems. Two of the HiFive projects managed by ARO have now ended.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Electronics Division.

A. Aluminum Gallium Nitride Nanowire Crystal Growth and Doping Techniques

Professor Zetian Mi, McGill University, Single Investigator Award

In FY15, Professor Mi's research team demonstrated advances in aluminum gallium nitride nanowires grown via molecular beam epitaxy techniques. Doping achievements were also made whereby hole conductivity was demonstrated at low temperatures where carriers usually "freeze-out" due to interband states where carriers reside until thermally activated. Nonetheless, it was found that carriers in nanowires can have significant densities at much lower temperatures – a property useful for low temperature optoelectronic devices. Lasing, in fact, was demonstrated in p-n junction nanowire "forests" of density 1e9 cm^{-2}. The nanowire structure consists of n-GaN (200 nm), n-AlGaN (90 nm), i-AlGaN (90 nm), p-AlGaN (90nm), and a thin p-GaN (10 nm) contact layer (see FIGURE 1). The growth temperature was 800 C. Samples with various Al/Ga flux ratios were grown and studied to achieve high efficiency emission in the wavelength range of 260 nm. The nanowire diameters are 65nm, with an average fill factor of 30% (considering the inversely tapered morphology). The lasing results focused on the operation at 77K with a linewidth of 0.3 nm and laser wavelength of 262.1 nm. However, subsequent results revealed lasing at room temperature as well at wavelengths both around 260 nm and 280 nm, with other wavelengths on the horizon.

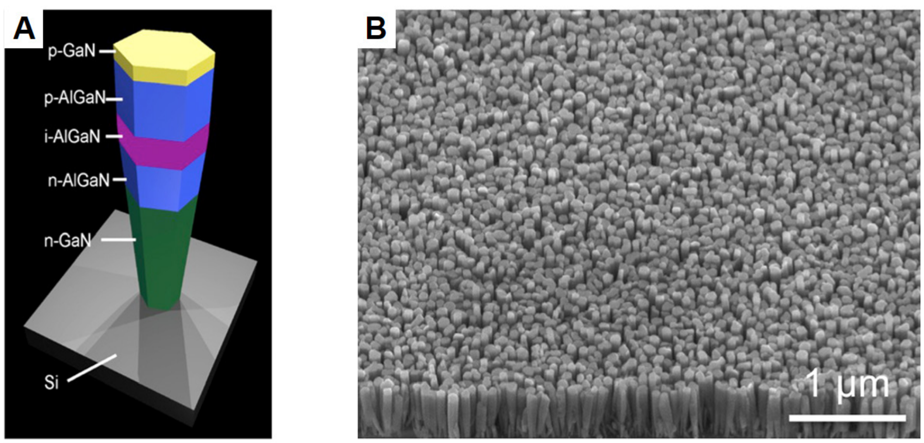

FIGURE 1

First ever UV-C semiconductor laser. (A) The schematic of the AlGaN nanowire laser structure; (B) The SEM (Scanning Electron Microscope) image taken at a 45 degree angle.

B. Fundamental Theoretical and Experimental Study of Nanoporation of Biological Cells

Professor James C. Hwang, Lehigh University, Single Investigator Award

The objective of this project, led by Professor James Hwang at Lehigh University, and involving co-PIs Professor X. Cheng and Professor M. Chang is to explore an innovative nano-electronic device concept for overcoming the challenges of conventional electroporation, and to precisely quantify the dynamics of electroporation as well as to detect and image the associated ion intake and release. Additionally, the innovative nano-electronic device concept is being explored for the precise application of nanosecond electric pulses to penetrate through the cell membrane and to investigate intracellular structures and functions. In FY15, the research team successfully demonstrated for the first time terahertz near-field sensing using a silicon CMOS chip (see FIGURE 2).

While awaiting the terahertz sensors to be designed, fabricated and tested as described in the above, the team also successfully demonstrated electroporation of biological cells as verified by optical microscopy. The demonstration used a previously designed coplanar waveguide, which was fabricated on a transparent substrate to trap a Jurkat human lymphoma cell for electroporation and optical verification (see FIGURE 3). With the experiments repeated over many cells, the percentage of cells porated and killed vs. the electroporation voltage at 10 MHz. The insets shows optical verification of cell poration by penetration of propidium iodide, a red fluorescence dye, into the cell, as well as cell vitality by the leakage of SYTO 9, a green fluorescence dye, out of the cell. The results show a narrow range of electroporation voltage so that statistically no cell was porated at 2.2 MV/m and all cells were porated at 2.7 MV/m. However, at this voltage, some cells began to die.

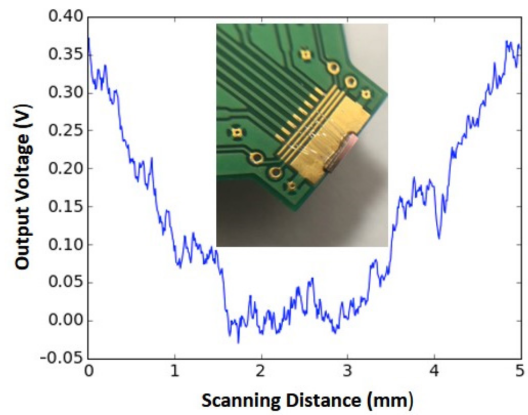

FIGURE 2

Preliminary results obtained by scanning the terahertz sensor across a silicon wafer in near field. The reflected terahertz signal was sensed through coherent mixing with the terahertz generator and the resulted frequency shift recorded as a voltage shift. (Inset) the 0.55 THz generator chip mounted on the edge of a printed circuit board.

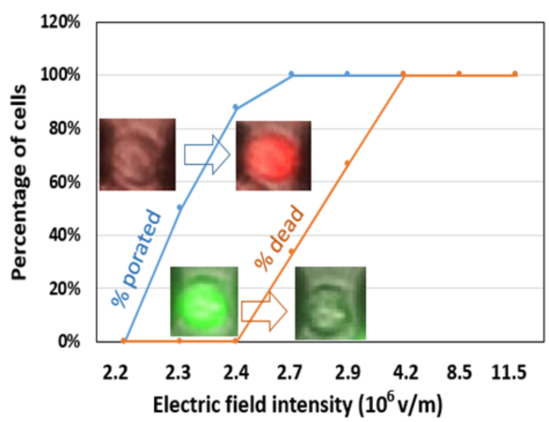

FIGURE 3

Electroporation of biological cells as verified by optical microscopy. Percentage of Jurkat human lymphoma cells porated (blue curve) and killed (orange curve) vs. electroporation voltage at 10 MHz. Insets show optical verification of cell poration by propidium iodide red dye and cell vitality by SYTO 9 green dye.

C. Small, Inexpensive Rapidly Tunable RF Filters for Integration In Communications and Radar Systems

Professor Robert York, University of California - Santa Barbara, Single Investigator Award

The goal of this research is to establish a uniquely systematic and comprehensive investigation of the anomalous loss resistance in field dependent (electrically tunable) high permittivity materials such as Barium Strontium Titanate (BST), exploiting recent developments in Molecular Beam Epitaxy (MBE) and MOCVD technologies. In FY15, the research team successfully demonstrated electrically tunable filters in epitaxial grown thin films of BST with quality factors (Q's) of over 200 at 1 GHz, which is about four times the best Q reported for other tunable dielectric filter research and with wide tuning range (see FIGURES 4-5). The tuning time for these filters is less than a microsecond, making them very attractive for frequency agile military radio and radar systems. The record quality factors were made possible by a systematic investigation of fundamental loss processes in BST structures and devices, with particular attention paid to film defects, metallization, metal etching, surface treatments, and passivation. So far, MBE is required to achieve the high quality films. Beyond the one-time expense of an MBE machine, the processing of these devices is very easy and inexpensive. Unlike MEMS filters, they can be integrated directly into a circuit without separate encapsulation. In general, they tune faster than MEMS filters, are much smaller, and have lower control voltages. They can handle significantly higher power than either MEMS or diode filters. The UCSB demonstration was with an interdigitated device structure, however the same understanding of the materials issues are expected to provide success for a parallel plate device. The interdigitated structure provides greater power handling capability, while the parallel plate structure allows smaller tuning voltages. These results point the way to much less expensive, rapidly tunable filters, phase shifters, linearization networks, and voltage-controlled oscillators, capable of handling high powers (or alternately capable of tuning with relatively low control voltages) for applications in military radios like JTRS, in satellite radios, in radar systems and in phased array communications and radar antennas. These research results formed the basis for a new SBIR topic on electrically tunable RF filters and varactors.

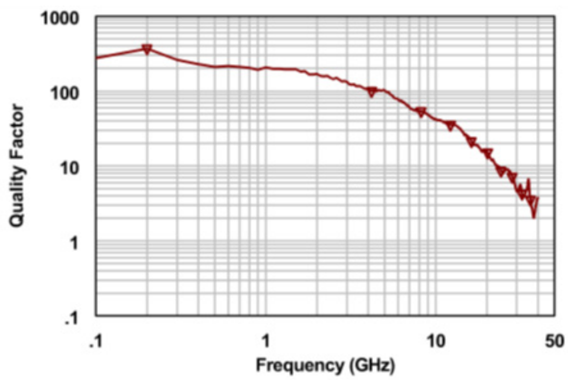

FIGURE 4

Quality factor of MBE grown BST interdigitated varactor from 100 MHz to 40 GHz. The plot shows the very high Q factor. The roll off with frequency is probably due to a resonance at 40 GHz, which can be moderated to some degree in the external circuit.

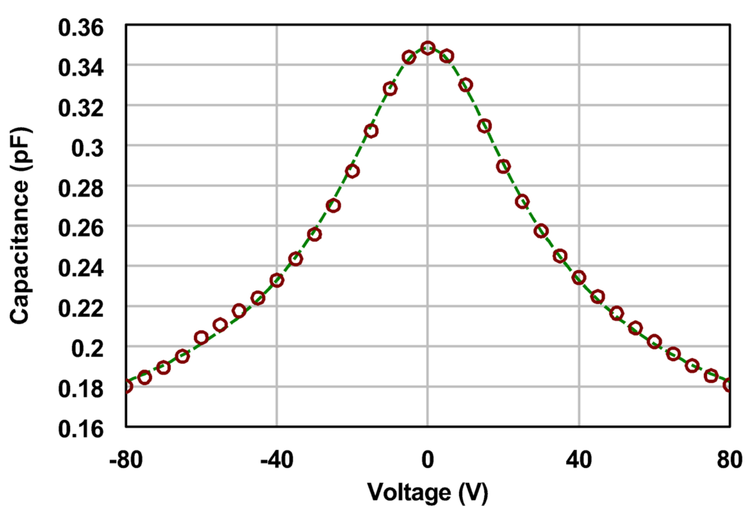

FIGURE 5

Tunability of MBE grown BST interdigitated varactor. The tenability was assessed at 1 GHz central frequency, showing a 2:1 turning range. The frequency change is proportional to the capacitance.

D. Ultrafast Carbon Nanotube-Oxide-Metal Tunnel Diodes
Professor Baratunde Cola, Georgia Tech Research Corporation, YIP Award

The objective of this work is to demonstrate infrared and optical response in a carbon nanotube-oxide-metal rectenna which is a combination of a rectifying diode and an antenna. Microwave rectennas have reached power conversion efficiencies of over 80%, but traditional rectenna structures in the visible regime face an RC time constant limitation that precludes useful operation. This project uses an innovative geometry involving multiwalled carbon nanotubes (MC) in a MC-insulator-metal arrangement (MC-I-M). In this arrangement the capacitance of a single tip is very small (~ 2 aF) and so the overall RC time constant is small enough to allow optical rectification (see FIGURE 6). Note that the R in the time constant is the effective resistance between the antenna resistance and the diode resistance which are in parallel. Unfortunately, there is a vast difference between the diode resistance which is very high and the antenna resistance so only a small amount of the energy can couple to the diode. However, it turns out that each carbon nanotube is optically coupled to its neighbor, such that the power that is reflected from one diode is coupled into neighboring diodes. Even though the coupling ratio is small, the high density of carbon nanotubes may allow sufficient overall coupling. In FY15 Professor Cola was able to show a response in his rectenna which clearly indicated optical rectification from a laser at 532 nm as well as simulated solar radiation. This is the world's first demonstration of optical rectification from visible and solar light. Much more work needs to be done to improve the diodes for efficient rectification, as well as to develop low-cost fabrication techniques for multiwalled carbon nanotubes but this technique has the potential to become appealing for practical applications.

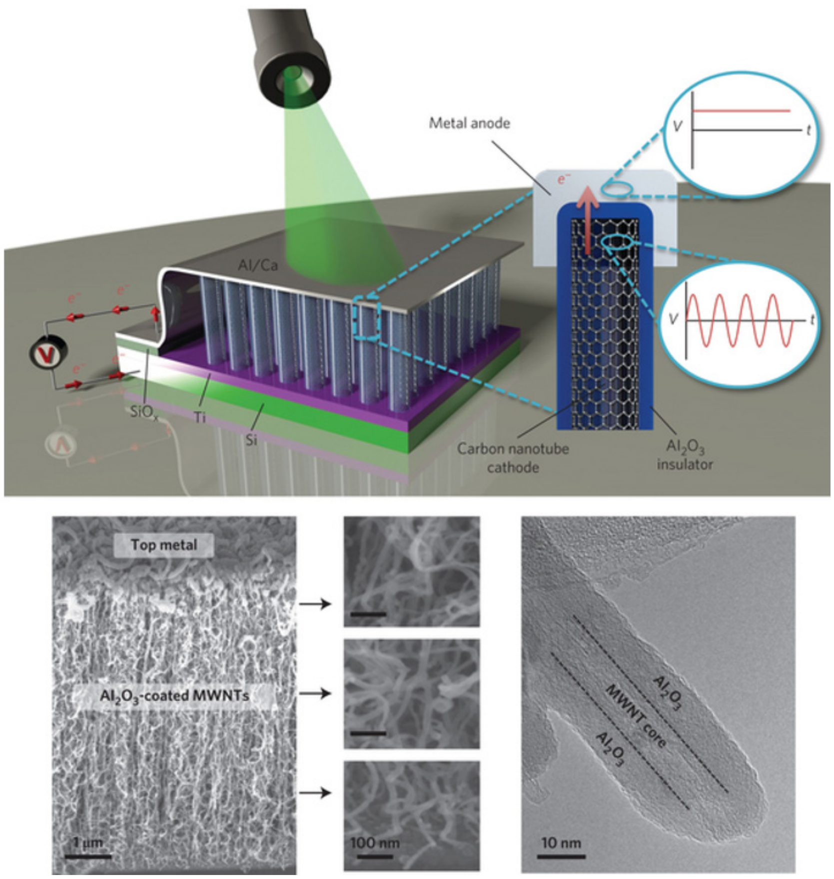

FIGURE 6

Schematic of the vertically aligned MC-I-M optical rectenna and SEM micrograph of a representative MC-I-M device.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Ultra-Narrow Linewidth Lasers via Slow-Light Silicon Microcavities

Investigator: Professor Amnon Yariv, California Institute of Technology, Single Investigator Award
Recipient: Telaris, Inc

Research reported upon in prior editions of ARO in Review, based on slow-light lasing effects in silicon microcavities has moved ahead for future applications in optical networking and lidar. Coherence, also related to how narrow a laser is the laser linewidth, is an important property for a number of optical propagation regimes. First, it allows more data channels to be co-propagated on a single waveguide simply due to the reduced channel spacing of narrower linewidth channels. Secondly, narrow linewidth lasers have implications for lidar (coherent ladar) whereby, the spatial resolution of the 3D image is directly related to it based on the improved coherence. And, finally, narrow linewidth lasers are useful in coherent photonics where the signals phase is accounted for as opposed to just its amplitude (polarization control is yet another degree of freedom).

The advancement, first made in a single investigator program, transitioned to industry where the proposed separation of the gain from longitudinal filtering was first studied. What was found over time was that very little overlap between the optical mode and the III-V semiconductor quantum well gain material was needed to lase the cavity. Thus, the control of the spontaneous emission can be made in a much lower loss silicon high-Q (or slow-light) microcavity, compared to the III-V semiconductors (see FIGURE 7). Bonding of the two forms a hybrid cavity with a SiO_2 spacer layer in between. Variations in the spacer layer thickness have a dramatic effect on the laser linewidth. Currently, achievements of several orders of magnitude were made over the single investigator results where linewidths of 60 kHz had once been the new gold standard, now less than 500 Hz has been estimated. Characterization and investigation of such narrow linewidth lasers is currently being pursued to assess the fundamental limits of the technology. This result is being transferred to a small company for fabrication of quantum noise-controlled lasers on a quarter-wafer scale for commercialization.

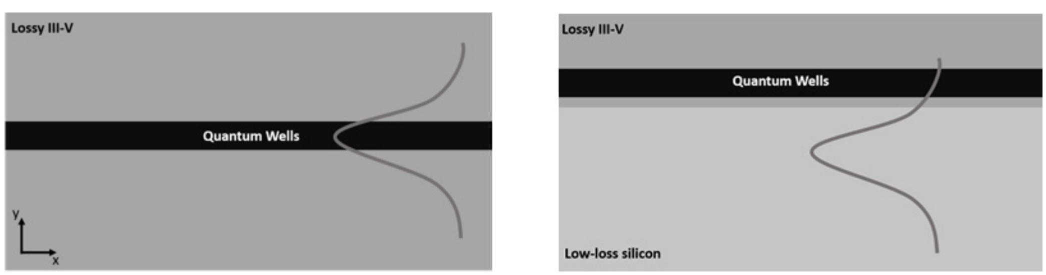

FIGURE 7

New laser design approach. (Left) Mode profile of a traditional III-V laser; (Right) Profile of a high-Q hybrid Si/III-V laser.

B. Enhanced Capabilities of Cochlear Implants

Investigator: Professor Les Atlas, University of Washington, Single Investigator Award
Recipients: Walter Reed Medical Center and Portland Veterans Administration Medical Center

The goal of this research is to investigate new techniques for the analysis of audio signals. In this research a new approach based on complementary correlation was applied to the modeling and analysis of the auditory system. The first application of the research was a significantly enhanced coding scheme for cochlear implants. The conventional approach to coding auditory information for cochlear implants is to filter the auditory signal into frequency bands, extract the Hilbert envelope of the signal within each band (similar to a rectification envelope), re-convolve the envelopes with the base frequencies of the (usually 4 or 8) channels of the cochlear implant, and apply the electrical signals to different positions in the cochlear nerve, simulating the tonotopic map generated in a healthy auditory system. The resulting signal processing by the brain can correctly interpret much of the original auditory signal, but some information is lost in this conventional modulation process, causing difficulty in distinguishing precise tones and in understanding speech in a noisy environment (the "cocktail party" problem). Professor Atlas' improvement relies on frequency down-converting the full signals within the initial filtered frequency bands and convolving them with the base frequencies in the channels of the cochlear implant. The better rendition of the information in the original signal results in significant improvement in musical recognition, tonal recognition, and understanding masked speech (See FIGURES 8–10).

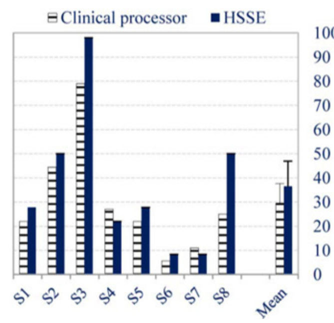

FIGURE 8

Comparison of melody recognition. Melody recognition comparing the conventional modulation for a cochlear implant ("clinical processor") vs Prof. Atlas's harmonic single sideband encoder ("HSSE"). "S1" - "S8" refer to different clinical trial subjects. The right hand vertical scale refers to percentage test melodies recognized.

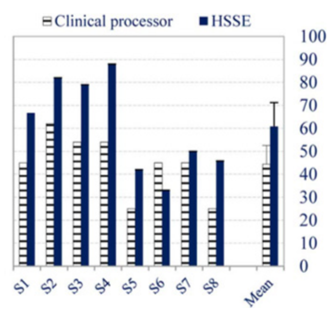

FIGURE 9

Comparison of timbre recognition. Timbre recognition comparing the conventional modulation for a cochlear implant vs Prof. Atlas's encoder.

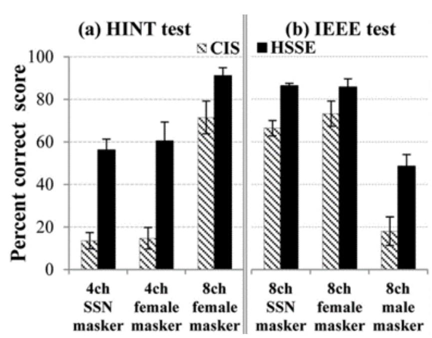

FIGURE 10

Comparisons of the ability of the conventional modulation for a cochlear implant ("CIS"), with Prof. Atlas's HSSE encoder, to distinguish speech in a noisy ("masked") environment. The "4ch" and "8ch" refer to the number of frequency channels in the cochlear implant. The maskers are a single tone ("SSN") and single female or male competing talkers. Two standard sets of test sentences were used, the "Hearing In Noise Test" (HINT) and an IEEE test set.

Two patents and a copyright have resulted, a cochlear implant algorithm and a spin-off algorithm for detecting objects in shipping containers based on vibrational analysis. A proposal for transitional funding is being considered by the Coulter Foundation, with university plans to license the technology. The cochlear implant algorithm has been delivered to Walter Reed and to the Portland VA Medical Center for evaluation and visits made to both to explain the algorithm and provide advice in its implementation.

C. Micromachined Probes for Measurement and Characterization of Terahertz Materials and Devices

Investigator: Drs. Robert Weikle, II and N. Scott Barker, Dominion MicroProbes, Inc., Army STTR
Recipients: DARPA and ARL-SEDD

The objective of this project is to create micromachined differential probes for characterization of devices in the 140 – 220 GHz and 220 – 330 GHz bands, as well as to engineer micromachined probe tip geometry and material to enable reliable and accurate characterization of terahertz devices with aluminum contact pads. Both of these efforts are widely recognized as critical tools for the advancement of terahertz science and engineering. Recently, there has been substantial progress in the development of CMOS-based millimeter- and submillimeter-wave integrated circuits, which often utilize aluminum differential probe pads. Above 110 GHz, however, the differential probes that are traditionally used to characterize these types of circuits do not exist. By developing millimeter- and submillimeter-wave differential probes with contacts engineered for aluminum pads, the results of this work facilitate the continued development of new terahertz devices and circuits.

A prototype micromachined differential probe is shown in FIGURE 11. The probe utilizes a radial stub waveguide transition to convert the waveguide mode to a rectangular coaxial mode. The coaxial transmission line, shown in the upper portion of Fig. 11b, carries the RF signal to the probe tip. At the probe tip, the coaxial mode is converted to microstrip, which feeds the input of a Marchand balun. The balanced output emerges on the back side of the probe tip, where a matching network utilizing a titanium thin-film resistor terminates the common-mode signal. Finally, vias are used to transition the balanced microstrip signal to GSGSG coplanar tip output. A proof-of-concept has been demonstrated in the 75 – 110 GHz band, and designs are currently being developed 140 – 220 GHz and 220 – 330 GHz bands. In addition, a 60 – 90 GHz design is being developed in response to a direct request to fill a commercial need.

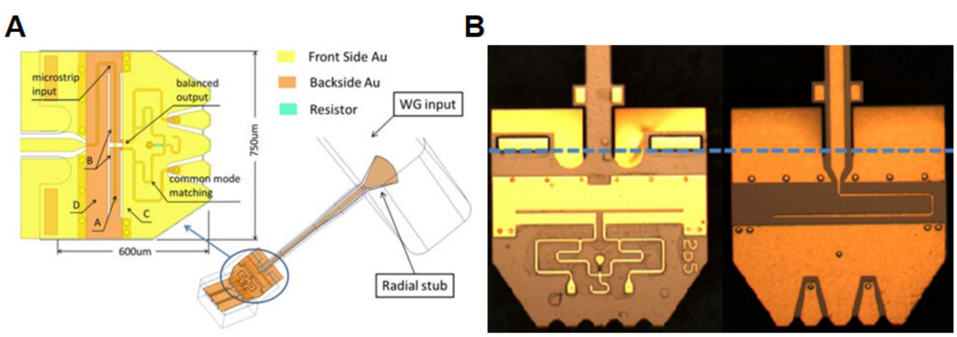

FIGURE 11

Micromachined integrated balun probe. (A) HFSS model, (B) left: back side showing balanced output and common-mode matching circuitry, right: front side circuitry showing single-ended input and 100 μm pitch GSGSG contacts at bottom.

This project is also investigating contact materials and geometries for micromachined aluminum probe tips (see FIGURE 12). The raised nickel wedges in the micromachined probe tip will allow the contact force of the probe to be concentrated over a smaller area, allowing it to break through the native oxide and protrude below the surface of the pad metallization. To create more uniform pressure across all three contacts, the silicon extents of the probe tip was modified to remove silicon near the outer contacts. This technique, which allows the outer contacts to be more compliant, has proven successful and has already been incorporated into DMPI's commercially available products.

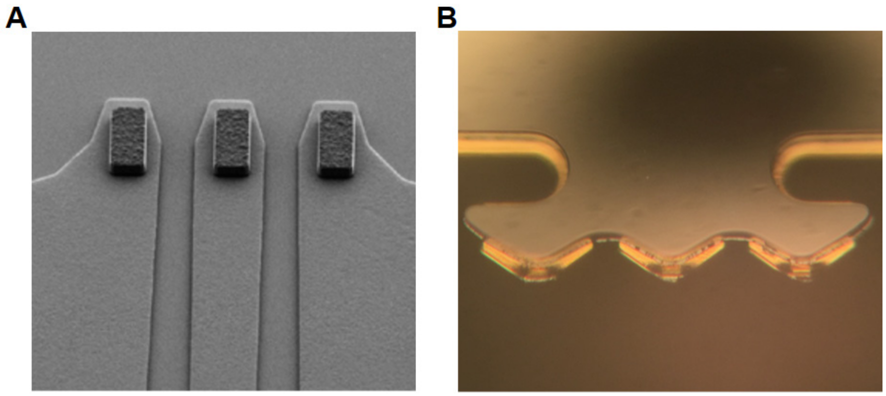

FIGURE 12

Engineered micromachined probe tip designs. (A) Raised nickel contacts for improved penetration into aluminum pads. (B) Etched reliefs in silicon provide more uniform pressure across the three tips, improving contact reliability for larger pitch probes.

This work is being performed by Dominion MicroProbes, Inc. (DMPI), in close collaboration with the University of Virginia. It has been transitioned to Dr. Dev Palmer of DARPA and Dr. Ali Darwish and Mr. Edward Viveiros of ARL-SEDD. Dr. Palmer is funding a phase III add-on effort to develop a terahertz active load-pull system based on the DMPI probe technology. An active load-pull system at terahertz frequencies will provide unprecedented capability for device characterization and enable development of new device concepts. Dr. Darwish and Mr. Viveiros will use the DMPI probes for on-wafer characterization of terahertz devices.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Betavoltaic Device with Enhanced Performance using WBG (Al)GaN Nanostructures

Professor Fatemeh Shadedipour-Sandvik, University of Albany-State University of New York, STIR Award

The objective of this work is to grow wide bandgap (Al)GaN nanostructures for increased current generation in III-Nitride based betavoltaic structures. GaN betavoltaic cells (and alloys with AlN) will have a large bandgap (3.6-6.2 eV) that can produce a larger open circuit voltage and higher electron-hole pair generation efficiency compared to smaller bandgap materials. III-Nitride semiconductors are also physically hard, radiation tolerant, and chemically inert making them ideal for their applications in harsh environments. However, there are several challenges with this material system including large leakage current created by the presence of recombination centers formed by dislocations, small currents due to the small surface area to footprint ratio of traditional configurations, and an inability to capture many of the carriers created by the ß-electrons outside of the depletion region. The novelty in this proposal is to use as-grown nanostructure pillars with a small width and high aspect ratio (see FIGURE 13). This will reduce the leakage current because of fewer defects in nanopillars. It will also significantly increase the available surface area of the np junction exposed to the ß-particles. In FY16 high quality p-type (Al)GaN will be epitaxially grown on Si or Sapphire substrates and beta-voltaic structures will be fabricated and tested. It is anticipated that the relevant characteristics will surpass those of planar p-(i)-n devices under similar doping density and alloy composition.

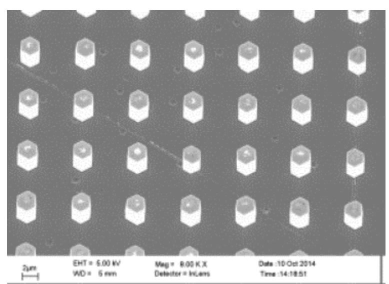

FIGURE 13

SEM image of high density of p-n+ GaN core-shell pillars epitaxially grown using selective area growth on n+ GaN template.

B. Low-Energy Tunable Self-Modulated Nanolasers

Professor Yeshaiahu Fainman, University of California at San Diego, STIR Award

The objective of this research is to design, fabricate, and characterize metallo-dielectric nanolasers. Researchers the University of California at San Diego are pursuing a new type of nanolaser that builds off of prior work completed under DARPA NACHOS program. It is anticipated that in FY16, the research team will produce the first wavelength tunable nanolaser (see FIGURE 14). Such an advancement is of high interest due to the potential use in on-chip and chip-to-chip optical interconnects where wavelength division multiplexing is highly desirable. Such multiplexing effectively creates multiple channels for data to independently traverse the same path What is needed is shown conceptually in the figure below; whereby, the size of the device is on par with the smallest single mode waveguides (about 100 nm) where such phenomena as the quantum confined Stark effect have never been explored. Free-carrier effects (or FCE) have known implications for such a regime where the external electric field will cause a redistribution of free carriers at the multiple quantum wells gain interface. Such FCEs will alter the optical mode which is critical to high-speed operation, output coupling, and efficient operation. Consideration of the FCEs will be made with optical pumping for this proof of concept. Both frequency and amplitude modulation regimes hold potential, and will be explored once the initial wavelength tenability concept has been measured. Further work could lead to electrically pumped wavelength tenability at very high rates; however, special consideration will need to be made to overcome thermal limitations of designs shown in the figure below. One possibility is to use coupled active nano-resonators to employ coupling from a forward biased to a reversed biased resonator where the absorption in the reversed-biased resonator effects the forward biased one through optical coupling. Energy consumption in such nanoscale resonators would hold great promise for future optical interconnect systems where wavelength tenability has usually relied on parametric processes such as four-wave mixing (FWM) that require high intensity light.

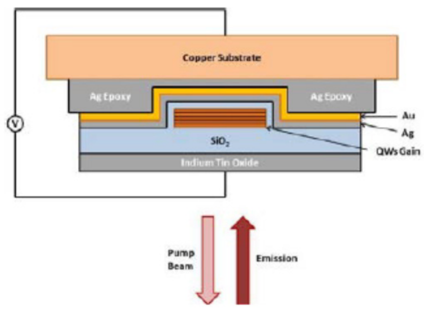

FIGURE 14

Schematic of the proposed tunable self-modulated optically pumped nanolaser.

C. New Regimes in THz Non-linear Interactions

Professor Xi-Cheng Zhang, University of Rochester, Single Investigator Award

The goal of this research is to explore non-linear interactions of ultrashort pulse THz radiation with gases and solid matter at unprecedented field strengths (1 - 10 MV/cm). There is very little research to date at these extremely high field strengths in the THz regime, although significant advances have been made in laser surgery, laser machining and processing of optical and electronic materials, medical imaging, femtosecond chemistry, and the table top generation of intense coherent UV and X-ray radiation, using femtosecond lasers at shorter wavelengths. The expectation is that new non-linear effects will be discovered from the interaction of ultrashort, extremely high field strength THz radiation with gaseous and solid matter. In FY16, Prof. Zhang is expected to complete development of a 10 MV/cm THz source and to begin experiments on coherent remote sensing phenomena in the atmosphere such as THz enhanced fluorescence and THz enhanced acoustic signatures, and of first ever measurements of non-linear responses from doped semiconductors, ferroelectrics, metamaterials, and composites, as well as novel new materials and biological materials.

D. THz Measures of Axion Electrodynamics and Exotic Superconducting Interfaces in Topological Insulator Films and Heterostructures

Professor N. Peter Armitage, Johns Hopkins University, Single Investigator Award

The objective of this research is to carry out a comprehensive experimental research effort into the electrodynamic response of topological insulators and their superconducting heterostructures using THz spectroscopy. Topological insulators (TIs) are newly discovered states of matter that host robust “topologically protected” surface states with spin-momentum locking. They are distinguished by topological properties of their quantum mechanical wave functions and not by broken symmetries. Their interesting physics is typically driven by strong spin-orbit coupling. These materials are interesting both in regards to fundamental physics as well as to their applications potential in devices for charge transport, photonic detectors, and topological quantum computation. The central part of this research is the use of unique low frequency “optical” probes in the THz range that are available in the PI’s group. Initial investigation by the PI has demonstrated that the electrodynamic response of topological insulator surface states is quantized (see FIGURE 15). This is a major result that goes back to original predictions in the early days of these materials. This quantization is a novel mangetoelectric effect in which an applied AC magnetic field induces an electric current. It is a 3D analog of the quantized off-diagonal conductivity found in 2D electron gases. In the case of topological insulators it appears in the form of a quantized Faraday rotation of a TI film under modest magnetic fields that is quantized in units of the fine structure constant. At the current level of experiment, the effect is quantized to about the 5% level. It is anticipated that in FY16 the research team will further refine the experiment to show the ultimate limits of this quantization.

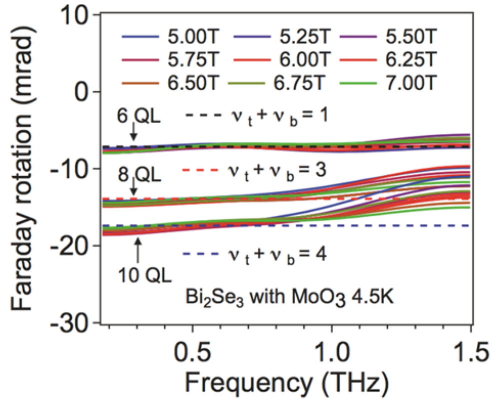

FIGURE 15

The electrodynamic response of TI surface states is quantized. Faraday rotation of 6 QL, 8 QL and 10 QL Bi_2Se_3/MoO_3 at 4.5 K with fields from 5 T - 7 T. A QL is one unit cell. The dashed lines are the expected quantized Faraday rotation calculation with different filling factors in units of the fine structure constant.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. William Clark, III
Division Chief
Program Manager, Electronic Sensing

Dr. Michael Gerhold
Program Manager, Optoelectronics

Dr. James Harvey
Program Manager (Acting), Electromagnetics and Radio-frequency Electronics

Dr. Joe Qiu
Program Manager (Acting), Nano- and Bio-Electronics

B. Directorate Scientists

Dr. David Stepp
Director (Acting), Engineering Sciences Directorate

Dr. April Brown (IPA)
Research Scientist

Mr. George Stavrakakis
Contract Support

C. Administrative Staff

Ms. Sade Sessoms
Contract Support

CHAPTER 6: LIFE SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2015* is to provide information on the programs and basic research supported by ARO in FY15, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Life Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY15.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Life Sciences Division supports research to discover and control the properties, principles, and mechanisms governing DNA, RNA, proteins, organelles, molecular and genetic systems, prokaryotic cells, eukaryotic cells, unicellular organisms, multicellular organisms, multi-species interactions, individual humans, and groups of humans. More specifically, the Division aims to promote basic research to elucidate the fundamental physiology underlying perception, cognition, neuro-motor output and non-invasive methods of monitoring cognitive states and processes during normal activity; basic research to understand antimicrobial resistance mechanisms; microbial community interactions including biofilm formation, cell-to-cell communications, population dynamics and host-pathogen/symbiont interactions; studies of organisms that are not culturable; studies of organisms at the single cell or mixed population (*e.g.*, metagenomic) level; studies of organisms that have adapted to grow or survive in extreme environments; identification and characterization of gene function, gene regulation, genetic interactions, gene pathways, gene expression patterns, mitochondrial regulation and biogenesis, nuclear and mitochondrial DNA replication, mutagenesis, oxidative stress, DNA repair, and regeneration; studies in structural biology, protein and nucleic acid structure-function relationships, molecular recognition, signal transduction, cell-cell communication, enzymology, cellular metabolism, and synthetic biology; and research to understand human behavior across different temporal, spatial and social scales. The results of this research will lay a foundation for future scientific breakthroughs and will enable new technologies and opportunities to maintain the technological and military superiority of the U.S. Army.

2. Potential Applications. Research managed by the Life Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the discoveries uncovered by ARO in the life sciences may provide new technologies for protecting the Soldier, for optimizing warfighter mental and physical performance capabilities, for creating new biomaterials, for advances in synthetic biology for energy production, intelligence, and bioengineering, and for new capabilities for predicting group behavior and change.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Life Sciences Division coordinates and leverages research within its Program Areas with many other agencies, including the Defense Threat Reduction Agency (DTRA), the Defense Advanced Research Projects Agency (DARPA), the Joint Improvised Explosive Device Defeat Organization (JIEDDO), the Army Natick Soldier Research Development and Engineering Center (NSRDEC), the U.S. Army Corps of Engineers (USACE), the Army Research Institute (ARI), the Army Medical Research and Materiel Command (MRMC), the Center for Disease Control (CDC), the National Institutes of Health (NIH), the Intelligence Advanced Research Projects Agency (IARPA), the Department of Homeland Security (DHS), the Army Criminal Investigation Laboratory (ACIL), the Federal Bureau of Investigation (FBI), the Office of Naval Research (ONR), and the Air Force Office of Scientific

Research (AFOSR). In addition, the Division frequently coordinates with other ARO and ARL Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, interactions with the ARO Chemical Sciences Division include promoting research to understand abiotic/biotic interfaces. The Life Sciences Division coordinates its research portfolio with the Materials Science Division to pursue the design and development of new biomaterials. The Life Sciences Division also coordinates extensively with the Mathematical Sciences Division to develop new programs in bioforensics. In addition the Division coordinates with the Materials Science and the Mechanical Sciences Divisions to understand the effects of blast on synapses. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

B. Program Areas

The Life Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY15, the Division managed research within these five Program Areas: (i) Genetics, (ii) Neurophysiology of Cognition, (iii) Biochemistry, (iv) Microbiology, and (v) Social and Behavioral Science. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Genetics. The scientific goals of this Program Area are to identify and characterize the mechanisms and factors that influence DNA stability and mutagenesis, gene expression, and genetic regulatory pathways in prokaryotes, eukaryotes, and eukaryotic organelles. This program also seeks to understand genetic instability at a population level. The program supports basic research on mitochondrial regulation and biogenesis, oxidative phosphorylation, oxidative stress, and the interactions and communication between the mitochondria and the nucleus. The Genetics Program also supports basic research to develop an empirical understanding of general mechanisms by which genomic, transcriptomic, and proteomic components respond to alterations in the population-genetic environment. A third area of emphasis is the identification, characterization, and modulation of genetic pathways and molecular cascades that determine the responses to stress and trauma.

This Program Area supports high-risk, high payoff basic research that has the potential to create new Army capabilities, to optimize warfighter mental and physical performance capabilities, to reduce the effect of PTSD, stress, and pathogens on warfighter readiness and Army capabilities, and to develop new sources of intelligence.

2. Neurophysiology of Cognition. The objective of this Program Area is to support non-medically oriented research to elucidate the fundamental physiology underlying perception, sensorimotor integration and cognition. Examples of research areas under this program can include the psycho-physiological implications of brain-machine interfaces that optimize auditory, visual and/or somatosensory function; display and control systems based on physiological or psychological states; measuring and modeling individual cognitive dynamics and decision making during real-world activity and uncovering the cellular biology of neuronal function.

This Program Area is divided into two major research thrusts: (i) Multisensory Synthesis and (ii) Neuronal Computation. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goals. Research in the Multisensory Synthesis Thrust aims to understand how the human brain functions in relation to the interaction of multisensory, cognitive and motor processes during the performance of real-world tasks. Basic research focused on mapping, quantifying and modeling distributed neural processes that mediate these features are being used to develop better understanding of the underlying bases of cognitive processes for eventual application to Soldier performance enhancement and improved human-machine symbiosis. Research in the Neuronal Computation Thrust is focused on understanding how living neuronal circuits generate desirable computations, affect how information is represented, show robustness to damage, incorporate learning and facilitate evolutionary change. Cell culture, brain slice and in vivo models are being used to develop better understanding of living neural networks for eventual application in Army systems that might include novel direct neural interfaces.

While these research efforts focus on high-risk, high pay-off concepts and potential long-term applications, current research may ultimately enable the development of neural biofeedback mechanisms to sharpen and differentiate brain states for possible direct brain-machine communication, identifying individual cognitive differences and new training paradigms for improved Soldier performance.

3. Biochemistry. The goal of this Program Area is to elucidate the mechanisms and forces underlying the function and structure of biological molecules. This research may enable the design and development of novel materials, molecular sensors and nanoscale machines that exploit the exceptional capabilities of biomolecules.

This Program Area supports two research Thrusts: (i) Biomolecular Specificity and Regulation, and (ii) Biomolecular Assembly and Organization. Within these Thrusts, innovative research efforts are identified and supported in pursuit of the vision of this program. Efforts in the Biomolecular Specificity and Regulation Thrust aim to identify the determinants of the specificity of molecular recognition and molecular activation/inactivation to modulate and control specificity and activity through protein engineering and synthetic biology approaches. Research in the Biomolecular Assembly and Organization Thrust aims to explore the fundamental principles governing biological self-assembly, to understand and control the relationships between molecular structure and biological material properties, and to identify innovative approaches to support biological activity outside of the cellular environment.

Research supported by this program promotes potential long-term applications for the Army that include biosensing platforms that incorporate the exquisite specificity of biomolecular recognition, nanoscale biomechanical devices powered by motor proteins, novel biotic/abiotic materials endowed with the unique functionality of biomolecules, drug delivery systems targeted by the activity and specificity of biomolecules, electronic and optical templates patterned at the nanoscale through biomolecular self-assembly, and novel power and energy systems that utilize biomolecular reaction cascades.

4. Microbiology. This Program Area supports research in fundamental microbiology and the bioengineering of microbial systems that can help advance needs in Soldier protection and performance. This Program Area is divided into two research Thrusts: (i) Microbial Survival under Environmental Stress and (ii) Analysis and Engineering of Microbial Communities. Research in the Microbial Survival under Environmental Stress thrust focuses on the study of the cellular and genetic mechanisms and responses that underlie microbial survival in the face of environmental stress. These stressors include extremes in temperature, pH, or salinity; the presence of antibiotics/antimicrobials and toxins including metals and toxic organic molecules; oxidative stress; and the depletion of specific nutrients. Research approaches include fundamental studies of microbial physiology and metabolism, cell biology, and molecular genetics that examine key cellular networks linked to survival, microbial cell membrane structure and the dissection of relevant critical signal transduction pathways and other sense-and-respond mechanisms; the dynamics of microbial-host interactions; and systems level, ecological and evolutionary approaches that examine the relationship and molecular communication within bacterial communities. Research in the Analysis and Engineering of Microbial Communities thrust focuses on the engineering of microorganisms toward biotechnological outputs and applications of interest to the Army. Engineered synthetic microbiological approaches are supported for studies in protein engineering, electromicrobiology, the production of biofuels and commodity chemicals and the bioremediation of toxins. Of joint interest with the ARO Biomathematics Program are research efforts the improve understanding of complex biological data sets representing microbiological systems.

While these research efforts focus on high-risk concepts, research supported by this program promotes a range of long-term applications for the Army, including strategies for detecting and classifying microbes, for controlling bacterial infections, for harnessing microbes to produce novel materials, to protect materiel, and/or to efficiently produce desirable commodities. In addition, understanding how microbes adapt is crucial for advancing studies in other fields, including genetics, environmental science, materials science, and medicine.

5. Social and Behavioral Science. The goal of this Program Area is to gain a better theoretical understanding of human behavior at all levels, from individuals to whole societies, for all temporal and spatial scales, through the development of mathematical, computational, simulation and other models that provide fundamental insights into factors contributing to human socio-cultural dynamics and societal outcomes (see FIGURE 1).

This Program Area is divided into two research Thrusts: (i) Predicting Human Behavior, and (ii) Complex Human Social Systems. The program supports research that focuses on the theoretical foundations of human behavior at various levels (individual actors to whole societies) and across various temporal and spatial scales. This includes, but is not limited to, research on the evolution and dynamics of social systems and organizations, human adaptation and response to both natural and human induced perturbations (*e.g.*, global climate change, mass migration, war, attempts at democratization, movements for social justice), interactions between human and natural systems, the role of culture and cognition in accounting for variations in human behavior, human decision-making under risk and uncertainty, the search for organizing principles in social systems, and the emergent and latent properties of dynamic social systems and networks. The research involves a wide range of approaches, including computational modeling, mathematical modeling, agent-based simulations, econometric modeling and statistical modeling, comparative-historical analyses, to name a few. The program also recognizes the fact that the building and validation of models in the social sciences is often limited by the availability of adequate and appropriate sources of primary data. A component of supported research includes the collection of primary data for model development and testing. The program also supports research to develop methodologies (*e.g.*, measurement, data collection, statistical methods, and research designs) that may provide an improved scientific understanding of human behavior.

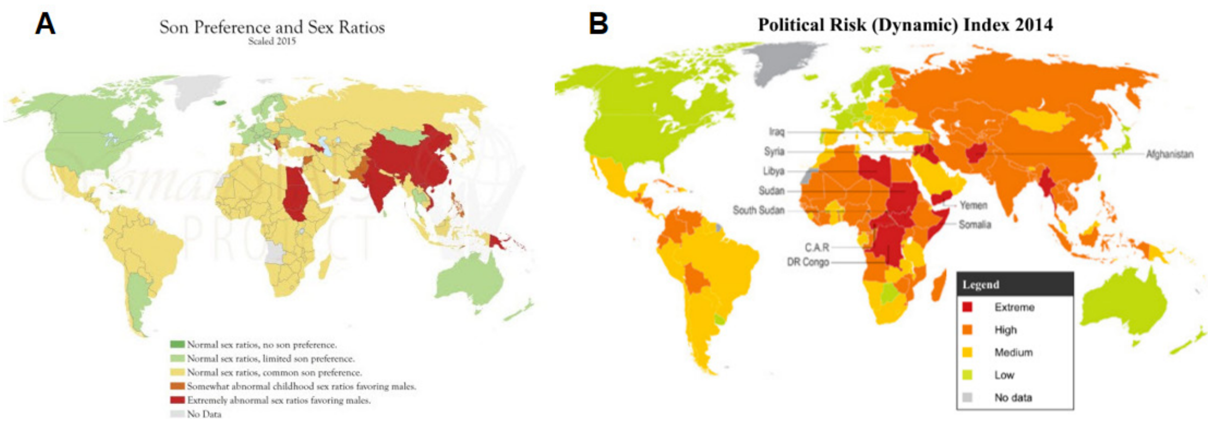

FIGURE 1

Correlation of population dynamics and sociopolitical instability. This research shows a correlation between (**A**) gender ratios in countries, and (**B**) risk of sociopolitical instability. The research reveals that in countries where males outnumber females, there may be a heightened risk of sociopolitical risk resulting from challenged male identities and a greater vulnerability of young males to recruitment by violent extremist organizations.

Research focuses on high-risk approaches involving highly complex scientific problems in the social sciences. Despite these risks, the research has the potential to make significant contributions to the Army through applications that will, for example, improve decision-making at various levels (policy, combat operations), create real-time computer based cultural situational awareness systems for tactical decision-making, increase the predictability of adversarial and allied intent, and produce integrated data and modeling in situ for rapid socio-cultural assessment in conflict zones and in humanitarian efforts.

C. Research Investment

The total funds managed by the ARO Life Sciences Division for FY15 were $105.9 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY15 ARO Core (BH57) program funding allotment for this Division was $8.0 million, which included a non-recurring annual increase of $0.8 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $8.2 million to projects managed by the Division. The Division also managed $71.9 million of Defense Advanced Research Projects Agency (DARPA) programs, $0.6 million for Minerva Research Initiative projects, and $2.9 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $1.6 million for contracts. The Institute for Collaborative Biotechnologies received $10.1 million. Finally, $2.7 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.1 million of ARO Core (BH57) funds, in addition to funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY15 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY15 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY15, the Division awarded 23 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Lawrence Appelbaum, Duke University; *Sensorimotor Function in Elite Soldiers and Athletes*
- Professor Danielle Bassett, University of Pennsylvania; *Dynamic Network Neuroscience: Probing Adaptation of Large-Scale Neural Circuits*
- Professor Mark Brynildsen, Princeton University; *Investigating the Metabolic Mechanisms of Bacterial Persistence*
- Professor Peng Chen, Cornell University; *Imaging Efflux Machineries for Metal Defense in Live Bacteria*
- Professor Natalie Elia, Ben Gurion University of the Negev; *Using Genetic Code Expansion For Nano-Scale Resolution Studies of the ESCRT Multiprotein Complex in Live Cells*
- Professor Andrew Ellington, University of Texas at Austin; *Design of Protein Biomaterials Through Tailored Shape and Packing Strategies of Patchy Particles*
- Professor Sharon Glotzer, University of Michigan - Ann Arbor; *Design of Protein Biomaterials Through Tailored Shape and Packing Strategies of Patchy Particles*
- Professor Caroline Harwood, University of Washington; *Protein Repair in Non-growing Bacteria*
- Professor Jay Hegde, Medical College of Georgia Research Institute, Inc.; *Neural Correlates of Recognizing Camouflaged Objects: A Human fMRI and EEG Study*
- Professor William Kalkhoff, Kent State University; *The Neurodynamics of Social Status*
- Professor David Kisailus, University of California - Riverside; *Organic-mediated Mineral Transport and Force Transduction in an Ultrahard Biological Composite*
- Professor Eric Kool, Stanford University; *Synthesis and Assembly of xDNA: Toward Unnatural DNA Nanostructures*
- Professor Beth Lazazzera, University of California - Los Angeles; *Increased Translation Error Rates and Long-term Survival*
- Professor Jin Montclare, New York University; *Patterned Protein and Hybrid Materials: Responsive "Chemomechanical" Shape-Shifters*

- Professor Anh-Tuan Nguyen, The College of New Jersey; *Measuring Neuronal Activity and Functional Connectivity in an In Vitro Model of Traumatic Brain Injury*
- Professor Aydogan Ozcan, University of California - Los Angeles; *Rapid Imaging, Detection and Quantification of Giardia lamblia Cysts using Mobile-phone Based Fluorescent Microscopy*
- Professor Dawn Robinson, University of Georgia Research Foundation, Inc.; *Computational Models of Cultural Meaning and Social Interaction*
- Professor Eric Schon, Columbia University Medical Center; *Investigation of the role of ApoE in Alzheimer Disease and Traumatic Brain Injury*
- Professor Brent Simpson, University of South Carolina; *The Social Structural Foundations of Reputation, Cooperation and Prosocial Behavior*
- Professor Michael Tobler, Kansas State University; *A Comparative Approach to Understanding the Physiological Effects and Processing of Hydrogen Sulfide*
- Professor Danielle Tullman-Ercek, University of California - Berkeley; *Engineering Nanoscale Protein Containers*
- Professor David Wolpert, Santa Fe Institute of Science; *Event-driven Game Theory for Predicting Dynamics of Social Systems*
- Professor David Yang, Georgetown University; *Data Analysis of Proteomes, Transcriptomes, Metabolomes from PTSD Samples*

2. Short Term Innovative Research (STIR) Program. In FY15, the Division awarded eight new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Bernard Brownstein, Washington University; *Regulation of Monocyte, Neutrophil, and T-cell Genes Involved in Coagulopathy as a Consequence of Trauma*
- Professor Bernard Brownstein, Washington University; *Burn injury induced regulation of WBC genes involved in coagulopathy*
- Professor Shelley Copley, University of Colorado - Boulder; *The Evolvability of Environmental Beta-lactamases*
- Professor Erika Eggers, University of Arizona; *Novel Mechanisms and Roles of Inhibition in Retinal Light Adaptation*
- Professor Mark Frye, University of California - Los Angeles; *Neural Mechanism for Reafference Rejection during Voluntary Saccades*
- Professor John Meitzen, North Carolina State University; *Validating a Mouse Tool for Analyzing Sex differences in Striatal Neurons and Pathologies*
- Professor Thomas Shea, University of Massachusetts - Lowell; *Does Insufficient Development Excitatory Activity Fail to Recruit Inhibitory Activity?*
- Professor Linlin Zhao, Central Michigan University; *Novel Role of PrimPol in Mitochondrial Genome Maintenance*

3. Young Investigator Program (YIP). In FY15, the Division awarded one new YIP project to drive fundamental research in areas relevant to the current and future Army.

- Professor Matthew Bolton, State University of New York at Buffalo; *Preventing Complex Failures of Human Interactive Systems with Erroneous Behavior Generation and Robust Task Behavior Patterns*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY15 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *7th Intl. Workshop on Advances in Electrocorticography (ECoG)*; Washington, DC; November 13-14, 2014
- *Sy-Bio Conference*; Dallas, TX; 25-26 March 25-26 2015
- *Twelfth Conference on the Foundations of Nanoscience*; Snowbird, Utah; 13-16 April 2015

- *7th biennial FASEB Science Research Conference on Ion Channel Regulation*; Big Sky, MT; 28 June - 3 July 2015
- *Foundations of Systems Biology in Engineering (FOSBE) 2015*; Boston, MA; 9-12 August 2015
- *21st International Conference on DNA Computing and Molecular Programming*; Harvard University; 16-21 August 2015
- *Technical Meeting of Biological Electron Transport*; RTP, NC; 15-16 September 2015

5. Special Programs. In FY15, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded nine new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Exploring Signaling Network Interactions Controlling Mouse and Salamander Limb Regeneration. This MURI began in FY09 and was awarded to a team led by Professor Ken Muneoka at Tulane University. The objective of this research is to identify and characterize signaling network interactions that control mouse and salamander limb regeneration.

The ultimate goal of this MURI is to establish the molecular-genetic foundation necessary for limb regeneration. The Mexican salamander is being used as a model organism. The investigators are using a comprehensive approach to document all gene transcripts that are modified during limb regeneration in this model organism. The researchers will use this data to develop a complete regeneration specific microarray chip that can be used to gather data from mathematical modeling of temporal changes in cellular transcriptomes associated with regeneration, in particular, the reprogramming of fibroblasts. The team will model regeneration in the mouse digit tip that is mediated by blastema formation. The modeling is expected to identify specific nodes during the injury response that control whether a wound heals via scar tissue or via reprogramming to form a blastema and eventually regeneration. In the long term, the results of this research could potentially be used to initiate regenerative therapeutics to be tested on amputated limbs in a rodent model.

2. Mechanisms of Bacterial Spore Germination. This MURI began in FY09 and was awarded to a team led by Professor Peter Setlow at the University of Connecticut Health Science Center. The objective of this research is to decipher the biological mechanisms that underlie heterogeneity of bacterial spore germination with an emphasis on the slow germinating population. This research is co-managed by the Mathematical Sciences Division.

Most bacterial spores readily and quickly germinate after being exposed to appropriate growth conditions, a small percentage do not. Within the population, individual spores may germinate days, weeks, or even months, with serious implications. In food processing, the presence of slowly germinating spores results in a need for harsh processing conditions, such as high pressure and temperature, leading to a loss of food quality and appeal. Medically, delayed germination can result in disease appearance after antibiotic therapy has been discontinued. This research team is using a combination of "wet lab" experiments and computational modeling to understand the fundamental mechanisms of spore germination. This research may ultimately lead to strategies for preventing bacterial spore germination that could be used in food processing and medically-relevant therapeutic technologies, and for the enhancement of spore germination to be used in new methods of biofuel production.

3. Modeling Cultural Factors in Collaboration and Negotiation. This MURI began in FY09 and was awarded to a team led by Professor Katia Sycara at Carnegie Melon University. The objective of this MURI is to understand how cultural values, such as the highly-prized "sacred values," can shape the collaboration and negotiation process.

The team has made interesting discoveries in these studies, including the observation of certain values called "sacred values" that are considered as essential to the identity of a given social group, thereby leading members of the group to respond defensively when these values are seen to be challenged or threatened. One example of sacred values includes the observation that the Iranian nuclear program is treated as sacred by some Iranians, leading to a greater disapproval of deals that involve monetary incentives. In addition the team is exploring how humiliation may contribute to regulating relationships within Muslim countries. Humiliation seems to result in clashing behavioral tendencies that offer no regulatory strategies. Participants in the study motivated to change the status quo underestimated the extent to which the out-group moralized the domains of harm, care, fairness and justice. Further, participants motivated to maintain the status quo accurately identified that the out-group moralized harm, care, fairness and justice to the same extent that they themselves did. The investigators will replicate these studies in India and Israel/Palestine in the coming year.

4. Blast Induced Thresholds for Neuronal Networks. This MURI began in FY10 and was awarded to a team led by Professor David Meaney at the University of Pennsylvania. This research is jointly managed with the ARO Mechanical Sciences Division. The objective of this MURI is to understand the effects of a primary blast wave and how it can cause persistent damage to the nervous system and the brain at the meso- and micro-scale.

The research team will build and validate a model of the human brain/skull subject to blast loading and use this model to scale blast field conditions into cell culture and animal models. This research will develop multiscale blast thresholds for alteration of synapses, neuronal connectivity, and neural circuits (*in vitro* and *in vivo*) and will examine if these thresholds change for tissue and/or circuits in the blast penumbra. Finally, the researchers will determine the blast conditions necessary to cause persisting change in neural circuitry components (up to two weeks) and will correlate alterations in circuits to neurobehavioral changes following blast. This research should provide a basis for shifting defensive armor design efforts from defeating the threat based on material deformation, damage, and rupture, to mitigating the effects based on biological relevance. In addition the research may lead to medical applications for treating neurotrauma and in regenerative medicine.

5. Prokaryotic Genomic Instability. This MURI began in FY10 and was awarded to a team led by Professor Patricia Foster at Indiana University. The objective of this research is to identify and extract the mathematical signatures of prokaryotic activity in DNA.

The investigators are characterizing fundamental parameters in the microbial mutation process in a superior model system, including both cell-mechanistic and evolutionary components. The research is a comprehensive effort with strong experimental and computational components. The team will determine the contribution of DNA repair pathways, cellular stress, and growth conditions on the mutation rate and mutational spectrum of *E. coli* using whole genome sequencing over the course of strain evolution. The team is extending this analysis to a panel of twenty additional eubacterial species. To understand the forces that define short-term and long-term evolutionary mutation patterns, a new class of population-genetic models will also be developed. The investigators will include mutant strains with known deficiencies in genome maintenance. Parallel analyses in such strains will produce larger data sets that define, by comparison to wild type strains, the contribution of each repair pathway to the overall mutational spectrum. Mutational changes characteristic to specific environmental conditions/stresses/genotoxicants can be analyzed in the context of the mutational signatures of individual repair pathway throughout the genome. Overall, the proposed research presents an unprecedented opportunity to uncover patterns of mutational variation among prokaryotes. The approach is unique in that the investigators are using a comprehensive whole-genome, systems-biology approach to characterize and understand DNA instability at a whole-genome level, across a comprehensive range of prokaryotes.

6. Translating Biochemical Pathways to Non-Cellular Environment. This MURI began in FY12 and was awarded to a team led by Professor Hao Yan at Arizona State University. This MURI is exploring how biochemical pathways could potentially function in a non-cellular environment.

Cells provide a precisely organized environment to promote maximum efficiency of biochemical reaction pathways, with individual enzymatic components organized via multisubunit complexes, targeted localization in membranes, or specific interactions with scaffold proteins. The eventual translation of these complex pathways to engineered systems will require the ability to control and organize the individual components outside of the natural cellular environment. Although biological molecules have been successfully attached to inorganic materials, this process often requires chemical modification of the molecule and can restrict its conformational freedom. An alternative approach to maintain biological activity outside of the cell, while preserving conformational freedom, is to encapsulate enzymes within specialized materials or structures. Unfortunately, surface patterning of current encapsulating agents has not achieved the precision required to replicate the organizational capabilities of the cell.

The objective of this research is to develop the scientific foundations needed to design, assemble, and analyze biochemical pathways translated to a non-cellular environment using 3D DNA nanostructures. The MURI team is using DNA nanostructures to direct the assembly of selected biochemical pathways in non-cellular environments. The focus of this research is to develop the scientific foundations needed to translate multi-enzyme biochemical reaction pathways from the cellular environment to non-biological materials. The ability to translate biochemical reaction pathways to non-cellular environments is critical for the successful implementation of these pathways in DoD-relevant technologies including responsive material systems, solar cells, sensor technologies, and biomanufacturing processes.

7. Evolution of Cultural Norms and Dynamics of Socio-Political Change. This MURI began in FY12 and was awarded to a team led by Professor Ali Jadbabaie at the University of Pennsylvania. This MURI is exploring the cultural and behavioral effects on societal stability.

Recent events involving the diffusion of socio-political change across a broad range of North African and Middle Eastern countries emphasize the critically important role of social, economic and cultural forces that ultimately affect the evolution of socio-political processes and outcomes. These examples clearly demonstrate that radically different outcomes and chances for conditions of state stability result from the different institutional frameworks within these countries. It is well established in the social sciences that change in or evolution of institutions depends on the behavior patterns or culture of the people involved in them, while these behavior patterns depend in part on the institutional framework in which they are embedded. This dynamic interdependence of culture and institutional change means that the modeling of societal stability requires the coupling of individual modeling approaches describing such issues as trust and cooperation with models describing institutional dynamics.

The objective of this MURI is to develop fundamental theoretical and modeling approaches to describe the complex interrelation of culture and institutions as they affect societal stability. The research team is extending the cultural approaches from application to individuals, families, and villages, to address stability of the larger social group. The models developed in this MURI may ultimately provide guidance in data collection and analysis of data on local populations that can provide planners with models to anticipate the second or third-order ramifications of actions that impact local populations.

8. Simultaneous Multi-synaptic Imaging of the Interneuron. This MURI began in FY12 and was awarded to a team led by Professor Rafael Yuste at Columbia University. The research team is exploring how individual neurons act as computational elements.

Interneurons are highly networked cells with multiple inputs and outputs. It has been to date impossible to record all the inputs and outputs from even a single living interneuron with synaptic levels of resolution in a living brain. While there is information on the morphological, physiological, and molecular properties of interneurons as a class and on their general synaptic connections, there is still little direct information on the functional roles of individual interneurons in cortical computations, and especially not on how each synapse relates to all the others within a single cell. Coupled with tagging via fluorescent molecules and/or chromophores and genomic modifications to control co-expression, electro-optical imaging may provide a solution, due to its ability to achieve subwavelength resolution across a relatively wide field of view.

The objective of this research is to explain and quantitatively model the entire set of neurotransmitter flows across each and every individual synapse in a single living interneuron, with experimental preparations ranging from cell culture systems through model neural systems. The research team will use genetically-engineered mice expressing specific labels in specific interneurons, high-throughput electron microscopy, and super-resolution imaging techniques to reveal the connectivity and the location of the synapses. This research may ultimately provide models that predict the information transitions and transformations that underlie cognition at the smallest scale where such activity could take place. These models could revolutionize the understanding of how human brains instantiate thought, and may lead to applications such as neural prostheses.

9. Artificial Cells for Novel Synthetic Biology Chassis. This MURI began in FY13 and was awarded to a team led by Professor Neal Devaraj at the University of California - San Diego. The goal of this MURI is to understand how biological and biomimetic synthetic cellular elements can be integrated to create novel artificial cells with unprecedented spatial and temporal control of genetic circuits and biological pathways. This research is co-managed by the Life Sciences and Chemical Sciences Divisions.

The field of synthetic biology aims to achieve design-based engineering of biological systems. Toward this goal, researchers in the field are identifying and characterizing standardized biological parts for use in specific biological organisms. These organisms serve as chassis for the engineered biological systems and devices. While single-celled organisms (e.g., bacteria, yeast) are typically used as synthetic biology chassis, the complexity of even these relatively simple organisms presents significant challenges for achieving robust and predictable engineered systems. A potential solution is the development of minimal cells which contain only those genes and biomolecular machinery necessary for basic life. Concurrent with recent advances toward minimal biological cells, advances have also been made in biomimetic chemical and material systems, including synthetic enzymes, artificial cytoplasm, and composite microparticles with stable internal compartments. These advances provide the scientific opportunity to explore the integration of biological and biomimetic elements to generate an artificial hybrid cell that for the first time combines the specificity and complexity of biology with the stability and control of synthetic chemistry.

The objective of this MURI is to integrate artificial bioorthogonal membranes with biological elements to create hybrid artificial cells capable of mimicking the form and function of natural cells but with improved control, stability, and simplicity. If successful, these artificial cells will provide a robust and predictable chassis for engineered biological systems, addressing a current challenge in the field of synthetic biology that may ultimately enable sense-and-respond systems, drug-delivery platforms, and the cost-effective production of high-value molecules that are toxic to living cells (e.g., alternative fuels, antimicrobial agents).

10. Force-activated Synthetic Biology. This MURI began in FY14 and was awarded to a team led by Professor Margaret Gardel at the University of Chicago. The goal of this MURI is to understand the mechanisms by which biochemical activity is regulated with mechanical force and reproduce the mechanisms in virtual and synthetic materials. This research is co-managed with the Materials Science Division.

A critical aspect of synthetic biology systems is the targeted and controlled activation of molecules affecting biological function. Molecules can be activated by a variety of different signals, including chemical, optical and electrical stimuli, and synthetic biological circuits responsive to each of these stimuli have been successfully assembled. In recent years, the ability of mechanical force to serve as a biological signal has emerged as a unique and unexpected facet to biological activation. The rapidly growing field of mechanotransduction is beginning to reveal an extraordinary diversity of mechanisms by which mechanical forces are converted into biological activity. This field has been heavily influenced and driven through ARO-funded research, including a prior MURI.[1] Despite these rapid advances, mechanophores have never been incorporated into advanced synthetic material. This research area provides an exceptional opportunity to integrate biological activation by mechanical force into the growing toolbox of synthetic biology, and to establish unprecedented paradigms for the incorporation of highly specific force activation and response into new materials.

The objective of this research is to elucidate the molecular mechanisms by which living cells regulate intracellular biochemical activity with mechanical force, to reproduce and analyze these force-activated phenomena in synthetic and virtual materials, and to design and exploit optimized synthetic pathways with force-activated control. If successful, this research may dramatically influence future advances in engineered biological systems, materials synthesis and fabrication, and force-responsive and adaptive bio-mimetic material systems.

[1] Potisek SL, Davis DA, Sottos NR, White SR, Moore JS. (2007). Mechanophore-linked addition polymers. *J Am Chem Soc*.129:13808-9.
Davis DA, Hamilton A, Yang J, Cremar LD, Van Gough D, Potisek SL, Ong MT, Braun PV, Martínez TJ, White SR, Moore JS, Sottos NR. (2009). Force-induced activation of covalent bonds in mechanoresponsive polymeric materials. *Nature*. 459:68-72.
Lenhardt JM, Ong MT, Choe R, Evenhuis CR, Martinez TJ, Craig SL. (2010). Trapping a diradical transition state by mechanochemical polymer extension. *Science*. 329:1057-60.
Burnworth M, Tang L, Kumpfer JR, Duncan AJ, Beyer FL, Fiore GL, Rowan SJ, Weder C. (2011). Optically healable supramolecular polymers. *Nature*. 472:334-7.

11. **Innovation in Prokaryotic Evolution.** This MURI began in FY14 and was awarded to a team led by Professor Michael Lynch at Indiana University - Bloomington. The goal of this MURI is to model evolution in nutrient-deprived bacterial cultures, and then characterize changes in the genetic, metabolic, and social networks to create models that reflect the complexities of group evolution.

Classical Darwinian evolution selects for individuals that are better than others of their species in critical areas associated with reproductive fitness. For example, giraffes are selected for longer necks and cheetahs are selected for running speed. Similarly, single-celled organisms growing in rich media are selected for their ability to reproduce more quickly. In contrast, organisms that have run out of food can no longer simply improve at what they are already able to do; they are forced to innovate new methods to exploit previously untapped resources. In times of scarcity, even unicellular organisms rapidly evolve into complex societies with assorted subpopulations formed with unique and specialized skills. It is no longer an effective strategy to grow faster during starvation. In short, evolution during lean times requires the group to evolve as a whole, as each individual competes, cooperates, and depends on other members of the group.

The objective of this research is to develop a model of evolution in isolated independent cultures of organisms that are starving for months or years, and then model change in the genetic, epigenetic, transcriptomic, proteomic, metabolomic, and social networks to create experimentally-validated, mathematically-rigorous, and predictive models that accurately reflect the real complexities of group evolution. In the long term, the results of this research may lead to new applications for safer, economical food and water storage, new mechanisms to control and kill pathogens that will impact wound healing, diabetes, heart disease, dental disease, and gastrointestinal disease.

12. **Imaging and Control of Biological Transduction using Nitrogen Vacancy Diamond.** This MURI began in FY15 and was awarded to a team led by Professor Ronald Walsworth at Harvard University. The goal of this MURI is to further develop nitrogen vacancy nanodiamonds as non-biological quantum sensors and engineer a biological interface for actuating biological processes. This research is co-managed with the Physics Division.

The nitrogen vacancy center lattice defect in diamond nanoparticles (NV-diamond) can retain activity in biological environments. Current applications of NV-diamond include quantum computing, nanoscale magnetometry, super-resolution imaging and atomic scale magnetic resonance imaging. These state of the art applications involve NV-diamonds implanted in substrates; however recent breakthroughs have allowed isolated nano-diamond particles to be used as biosensing intracellular quantum probes for thermometry and bacterial tracking as well as extracellular quantum probes of ion channel operation. A key reason for NV-diamond sensitivity, including in the emerging biosensing applications, is that the spectral shape and intensity of optical signals from NV-diamond are sensitive to external perturbation by strain, temperature, electric fields and magnetic fields. Biological sensory transduction relies upon highly evolved ion channel-based mechanisms that involve transducing environmental energy into a bioelectrical signal for intercellular communication. The recent demonstrations of NV-diamond's extreme sensitivity and localization now provide new research opportunities for transitioning NV-diamonds from passive sensors to novel biophysical interfaces whose perturbed energy emission can be used as a signal to control or modify sensory transducer molecular physiology and intra- and inter-cellular signaling.

This multidisciplinary project four closely-coupled aims: (1) to optimize nitrogen vacancy nanodiamond synthesis, (2) to realize stable, biocompatible nanodiamond surface functionalizations, (3) to advance nitrogen vacancy sensitivity to chemical and biological systems and (4) to enable nitrogen vacancy-based manipulation of biological transduction. Systematically studying the integration of nitrogen vacancy nanodiamonds with reconstituted or native ion channels will lead to greater understanding but will, more importantly, create a new paradigm for exogenous control of biological transduction events and the ability to uncover fundamental mechanisms with unprecedented spatial and temporal resolution. The outcome from this endeavor will lead to significant scientific breakthroughs in understanding how to develop and control quantum systems capable of interfacing with, and controlling, biological systems. If successful, the research efforts may improve future Army capabilities ranging from advanced artificial intelligence systems, early diagnosis and effective treatment of neurological disorders at the cellular and network levels, novel human-machine interfaces, and antidotes to neurotoxins, pathogens, and other diseases.

C. Small Business Innovation Research (SBIR) – New Starts

Research within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY15, the Division managed two new-start Phase II SBIR contracts, in addition to active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY15 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY15, the Division managed three new-start Phase I STTR contracts, in addition to active projects continuing from prior years. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY15 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY15, the Division managed three new ARO (Core) HBCU/MI projects and 12 new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The PECASE winners for each year are typically announced by the White House at the end of the calendar year. However, the FY13-FY15 PECASE recipients had not yet been announced by the end of FY15. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY15, the Division managed 12 new DURIP projects, totaling $2.3 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. University Affiliated Research Center (UARC): Institute for Collaborative Biotechnologies (ICB)

The ICB is managed by ARO on behalf of the Army and is located at the University of California, Santa Barbara (UCSB), in partnership with the Massachusetts Institute of Technology (MIT), the California Institute of Technology (Caltech) and industry. The scientific objective of the ICB is to investigate the fundamental mechanisms underlying the high performance and efficiency of biological systems and to translate these principles to engineered systems for Army needs. Through research and strategic collaborations and alliances with Army laboratories, Research, Development and Engineering Centers (RDECs), and industrial partners, the ICB provides the Army with a single conduit for developing, assessing and adapting new products and biotechnologies for revolutionary advances in the fields of biologically-inspired detection, materials synthesis, energy generation and storage, energy-dispersive materials, information processing, network analysis and neuroscience. A total of $10.1 million was allocated to the ICB in FY15, which was the second year of the contract that was amended in FY14 for the next five-year period. Of these FY15 funds, $8.8 million was allocated for 6.1 basic research and $1.3 million was allocated for four 6.2 projects.

In FY15, the ICB supported 56 faculty members, 89 graduate students, and 58 postdoctoral fellows across 15 departments at UCSB, Caltech and MIT. The research falls into six Thrusts: (i) Systems and Synthetic Biology, (ii) Control and Dynamical Systems, (iii) Photonic and Electronic Materials, (iv) Cellular Structural Materials, (v) Biotechnology Tools, and (vi) Cognitive Neuroscience. Detailed descriptions of each core research Thrust and corresponding projects are available at the ICB program website (*http://www.icb.ucsb.edu/research*). A U.S. Army Technical Assessment Board and an Executive Steering Board biennially review the ICB research portfolio, assessing the project goals and accomplishments and set goals for the coming year.

I. DARPA Reliable Neural-Interface Technology (RE-NET) Program

The goal of this program is to develop high performance and clinically viable in-vivo neural interfaces to control dexterous functions made possible with advanced prosthetic limbs, enabling service members with amputations to return to active duty and improve their quality of life. ARO Life Sciences co-manages projects in the Reliable Peripheral Interfaces (RPI) focus area, which involves the design, fabrication, testing, and analysis of new materials and technologies to demonstrate substantial improvements in reliability and quantity of peripheral motor-signal information available to drive a neuroprosthetic device. One approach supported through this program involves the translation of surface or intramuscular electromyogram activity to drive neuroprostheses via the recognition of specific electrical activity patterns from residual muscles. This ‘intended movement’ information enables unprecedented control of robotic limbs. Another approach is exploring the design of a sensory feedback interface from the prosthetic fingers to the user’s skin to enable intuitive touch feedback.

J. DARPA Enabling Stress Resistance Program

The goal of this program, co-managed by the Life Sciences Division and DARPA, is to create a comprehensive, quantitative description of the impact of stress on the brain. This research seeks to leverage cutting-edge technologies and recent advances in molecular neurobiology, neuroimaging and molecular pathway modeling as applied to animal models of acute and chronic stress. The objective of this research is a proactive approach to stress mitigation, starting with development of a comprehensive understanding of the complex effects of multiple stressors on the brain. The program has the ultimate goal of the development and implementation of cognitive, behavioral, and/or pharmacological interventions that will prevent the deleterious effects of stress on the brain. The investigators will pursue their objectives through the creation of research teams to thoroughly investigate the multiple physiological pathways and molecular mechanisms involved in the brain’s response to acute and chronic stress as well as physical, social, cognitive and affective stressors.

K. DARPA Stochastic Computing Machines Enabled by DNA Self-Assembly Project

The Life Sciences Division currently co-manages a DARPA project focused on creating stochastic computing machines using self-assembled DNA nanostructures. This joint project aims to demonstrate the feasibility of a new class of computing machine that is physically implemented by DNA self-assembly and molecular-scale devices. The computing machine will be based on digital stochastic state machines, unlike traditional digital circuits, which are based around deterministic finite state machines. The planned computing machine has potential to deliver improved performance at vastly reduced power and size by using architectures that are implemented using nanoscale physical devices.

L. DARPA Systems-Based Neurotechnology for Emerging Therapies (SUBNETS) Program

The goal of this program is to create an implanted, closed-loop diagnostic and therapeutic system for treating, and possibly even curing, neuropsychological illness in humans. ARO Life Sciences co-manages SUBNETS projects focused on treatments to restore normal functionality following injury to the brain or the onset of neuropsychological illness. The major approach supported through this program involves clinical trials which will use current FDA-approved implantable intracranial recording devices in neurosurgical patients with psychiatric, epilepsy, movement disorder, and pain conditions in order to identify the corresponding 'signature' network-level brain activity aberrations in these patients. This knowledge will be applied towards a novel treatment strategy based upon a physiologically-defined computational model of neurological circuit function integrated into a closed-loop system. A complementary approach is to develop novel state-of-the-art technology for safe, but high spatiotemporal resolution recording and stimulation to multiple brain regions simultaneously for clinical application. This device platform will far exceed the capabilities of any technology platform ever created and will be available for experimental studies in non-human primates to obtain critical knowledge on mechanisms and will simultaneously inform human clinical studies to validate new recording/stimulation strategies for potential amelioration of human neurological and neuropsychiatric disorders.

M. Department of Defense Forensics and Biometrics Research and Development Program

The goal of this program, co-managed by the Life Sciences Division and DFBA, is to enhance the capability of forensic science and biometric applications for DoD customers both in traditional law enforcement/criminal justice purviews and in expeditionary environments. In FY15, five active projects were co-managed by ARO and DFBA under this program. One project is focused on statistical analysis of firearms and aims to develop a system to allow for examiner-independent evaluation of impressions generated by the discharge of a firearm using Integrated Ballistics Identification System (IBIS) data. In the expeditionary environment, the proposed system will provide a useful measure of match statistics, reducing time and potentially the need for a verification step, allowing a single examiner to make decisions on firearm comparisons. Another project aims to identify body fluid-specific gene transcripts and incorporate them into an RNA-based body fluid multiplex identification system. The proposed system will enhance forensic capabilities of DFBA and civilian law enforcement by conclusively identifying all forensically relevant biological fluids in a given sample. The proposed system will also be seamlessly compatible with current DNA typing technology by enabling co-extraction of both DNA and RNA from the same forensic sample. One effort will evaluate ground-, air- and satellite-based sensing technologies for their performance in human grave detection using an experimental study site in east Tennessee, with the main data focus on LIDAR and spectral imaging. The development of remote methods to locate clandestine gravesites will increase gravesite detections per year, reduce recovery cost per individual, and enable the DoD to closely monitor additional gravesites in non-permissive environments, thereby maintaining the grave's chain of custody. Another effort will develop a Next Generation Sequencing-based autosomal short tandem repeat (STR) allelotyping capability. The proposed platform will enable STR analysis and mitochondrial DNA to be analyzed concurrently, along with other genetic markers that can provide information on the physical characteristics and ancestry of an individual, providing enhanced forensic information to examiners. The final project is developing a set of algorithms and software tools to discover the make and model of a digital image's source device by forensically analyzing the image itself. If successful, this effort would provide a new capability to Army and DoD forensic examiners, as there is currently no scientific method available to make this determination.

N. DARPA Rapid Threat Assessment (RTA) Program

The goal of this program is to develop methods and technologies that can, within 30 days of exposure to a human cell, map the complete molecular mechanism through which a threat agent alters cellular processes. The program is co-managed by the Life Sciences Division, which involves participation and leadership in proposal evaluations, selections, monitoring, and site visits. Research challenges include developing tools and methods to detect and identify the cellular components and mechanistic events that take place over a range of times, from the milliseconds immediately following threat agent exposure, to the days over which alterations in gene and protein expression might occur. Understanding the molecular mechanism of a given threat agent would provide researchers the framework with which to develop medical countermeasures and mitigate threats. If RTA is successful, potential adversaries will have to reassess the cost-benefit analysis of using chemical or biological weapons against U.S. forces that have credible medical defenses.

O. DARPA Pathogen Predators Program

The goal of this program is to demonstrate that infections caused by drug-resistant bacterial pathogens and bacterial threat agents might be effectively treated with live predatory bacteria. The program is co-managed by the Life Sciences Division, which involves participation and leadership in proposal evaluations, selections, monitoring, and site visits. The program is focused on answering three fundamental questions about predatory bacteria: (1) Are predatory bacteria toxic to recipient organisms? (2) Against what pathogens are predatory bacteria effective? (3) Can pathogens develop resistance to predation? The potential use of live predatory bacteria as a treatment regimen for bacterial infection would represent a significant departure from conventional antibacterial therapies that rely on small molecule antibiotics.

P. DARPA Biological Robustness in Complex Settings (BRICS) Program

The goal of this DARPA program is to develop the fundamental understanding and component technologies needed to engineer biosystems that function reliably in changing environments. A long-term goal is to enable the safe transition of synthetic biological systems from well-defined laboratory environments into more complex settings where they can achieve greater biomedical, industrial and strategic potential. Within this program, the Life Sciences Division co-manages one project which seeks to develop new approaches to manipulate unculturable and undomesticated microbes through *in situ* genome engineering. These technologies have the potential to discover new genetically tractable microbes with novel manipulable capabilities for applications in agriculture, bioremediation, bioenergy, biodefense and health. This project further focuses on the development of a generalizable method to limit robustness of the genetic code using overlapping genetic recoding. The results from this genetic study will be useful as a defense against targeted efforts to inactivate a gene or pathway of interest or to remove the engineered safety mechanisms associated with a synthetic function.

Q. DARPA Hand Proprioception and Touch Interfaces (HAPTIX) Program

The goal of this program is to create a prosthetic hand system that interfaces permanently with the peripheral nerves in humans. ARO Life Sciences co-manages HAPTIX projects focused on tapping into the motor and sensory signals of an amputee's residual arm, allowing them to control and sense an advanced prosthesis via the same neural signaling pathways used for intact hands and arms. Direct access to peripheral nerves would allow users to move and receive sensation like a natural hand such that it creates a sensory experience so rich and vibrant that users would want to wear their prostheses full time. By restoring sensory functions, HAPTIX also aims to reduce or eliminate phantom limb pain, which affects about 80 percent of amputees. The program plans to adapt one of the prosthetic limb systems developed recently under DARPA's Revolutionizing Prosthetics (RP) program to incorporate interfaces that provide intuitive control and sensory feedback to users. These interfaces build on advanced neural-interface technologies being developed through DARPA's Reliable Neural-Interface Technology (RE-NET) program.

R. Minerva Research Initiative (MRI) Topic: Studies of Non-State Adversarial Organization, Ideologies, and Strategies

The objective of this MRI topic is to examine the relationship between trans-national terrorist ideologies and intergroup conflicts. Areas of particular interest include: the interaction between political dynamics on the ground and the goals and ideologies of non-state adversarial groups; the role of new media technologies in recruitment, radicalization, and de-radicalization in insurgent movements; the spread of insurgent ideologies across culturally diverse populations; and the role of non-rational decision making (e.g., values, morals, trust, belief and emotions) in the collective behavior in insurgent groups and how best to represent non-rational decisions in computational models of collective and group behavior. This research, if successful, will provide better understand the dynamics of non-state adversarial organizations, their underlying motivations and ideologies, how they organize, how they recruit and retain members, and how they evolve and adapt in the face of new challenges. In addition to overall network characterization, there is an urgent need to be able to locate the points of influence and characterize the processes necessary to influence populations that harbor terrorist organizations in diverse cultures as well as individuals who identify with terrorist group figures of note. A better understanding of neuro-cognitive systems responsible for the processing of socio-cultural and other environmental cues is crucial both to research and to a whole range of practical situations. The BAA for this

MRI topic was released in FY08, FY09, FY10, FY11, FY12, FY13, FY14. Project selection and funding began in FY09. There were nine active projects pursuing research under this topic in FY15.

S. Minerva Research Initiative (MRI) Topic: Science, Technology, Political, and Military Transformation in Asia, Eurasia, & Latin America

The objective of this MRI topic is to explore the social, cultural, and political characteristics and implications of trends and developments in growing military powers (e.g., China, Brazil, Russia), as well as in supporting technological and industrial sectors as they relate both to security policy and strategy and to the broader evolution of society. This research area utilizes a wealth of unclassified information, not generally known beyond a small circle of researchers, about military, technological and scientific development (including information that is published by governments in these states, but difficult for scholars outside of them to locate or access). Access to these data will facilitate research into trends in military and technology development and promise to provide valuable insights into the workings of an important and influential power. The coding of this data into a comprehensive relational database that will be made available to scholars beyond this project combined with the projects continued focus on building a community of researchers collectively engaged in understanding these aspects of modern international military development. The breadth and depth of topics offers insights into the dynamics and intersections of industry, science, technology, political governance, and social structures that shape modern military organizations and indicate why some countries emerge as military powers, while others remain stagnant. The research will inform a wide range of decisions relevant to national security and economic policy, from diplomacy to science and technology planning to military resource allocation. The BAA for this MRI topic was released in FY11, FY12, FY13, FY14. Project selection and funding began in FY12. There were seven active projects pursuing research under this topic in FY15.

T. Minerva Research Initiative (MRI) Topic: Security Implications of Energy, Climate Change, and Environmental Stress

The objective of this MRI topic is to establish new theories and models of societal response to external pressures that shape sociopolitical outcomes. Of particular interest are stressors related to environmental stressors. Until recently, most studies of these phenomena have focused on historical case studies and domain-specific policy development (*e.g.,* establishing policy on carbon footprint reduction, cross-national cooperation to manage water resources, developing policies to improve food security). In the last few years, social scientists began to quantitatively explore the intersection among these factors by asking how changes in the environment alter risk perception and human behavior, and affect the availability and distribution of essential resources (*e.g*., water, grains) and geomorphologic changes (*e.g.*, desertification). Affected societies experiencing these shifts must work to mitigate competition over increasingly scarce resources, which can otherwise contribute to the emergence of political and social unrest. In addition, worldwide increases in demand for nonrenewable energy and resource access have the potential to limit the ability of societies to sustain current economic and social standards of living. This MRI supports research that will contribute to fundamental understanding of the implications of these exogenous stressors from a global security perspective. This research will likely aid DoD decision-making in terms of the development of improved methods for identifying and anticipating potential hot zones of unrest, instability and conflict and help in strategic thinking about resource allocation for defense efforts and humanitarian aid. The BAA for this MRI topic was released in FY10, FY11, FY12, FY13, and FY14. Project funding and selection began in FY12. There were five active projects pursuing research under this topic in FY15.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Life Sciences Division.

A. Reprogramming Proteins and Enzymes for Transition Metal Catalysis

Professor Jared Lewis, University of Chicago, Single Investigator Award

Controlling the selectivity of chemical reactions and conducting these reactions in biological systems, where they could have a transformative impact, stand as key challenges in synthetic chemistry. Professor Jared Lewis at the University of Chicago is exploring artificial metalloenzymes (ArMs) as a potential route to achieve these goals by combining the reactivity of synthetic metal catalysts and the adaptability and efficiency of enzymes.

The overall goal of this project is to develop ArMs generated from protein or enzyme scaffolds and metal catalysts bearing reactive anchoring groups. Ensconcing metal cofactors within structurally defined yet genetically mutable protein scaffolds will provide exquisite control of reactivity. The impact of this control on catalysis will be studied, and ArMs will be evolved to promote challenging chemical transformations, including enantio-specific and site-specific C-H insertion reactions. Ultimately, these ArMs could enable chemistry typically conducted in the confines of flasks and reactors to operate in cells and living organisms.

In FY15, an ArM that catalyzes olefin cyclopropanation was created by covalently linking a dirhodium metal catalyst to a prolyl oligopeptidase enzyme (see FIGURE 2). Random mutagenesis of the enzyme scaffold was then used to improve the enantioselectivity of the reaction. Significantly, the ArM reduces the formation of reaction byproducts, including those resulting from the reaction of intermediates with water. This showed that an ArM can improve the substrate specificity of a catalyst and, for the first time, the water tolerance of a metal-catalyzed reaction, which is required for ArM-catalyzed C-H insertion. This scientific accomplishment was published in *Nature Communications* in July 2015. Given the diversity of reactions catalyzed by dirhodium complexes, it is anticipated that dirhodium ArMs will provide many unique opportunities for selective catalysis.

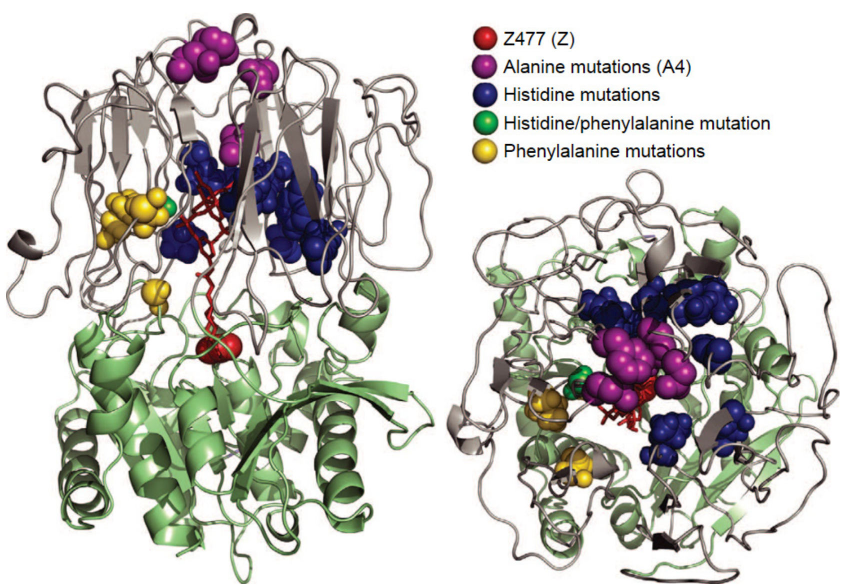

FIGURE 2

Structure of an Artificial Metalloenzyme (ArM). Homology model of *Pyrococcus furiosus* (*Pfu*) prolyl oligopeptidase (POP). The hydrolase domain is shown in green, the propeller domain is shown in gray. The metal cofactor linked at amino acid Z477 is shown in red. Sites of different mutations introduced into Pfu POP are shown as colored spheres.

Professor Lewis will build upon these results to explore the ability of the enzyme scaffold to impart similar selectivity to other metal complexes, as well as the potential to form ArMs *in vivo* that are active in catalysis. This project will provide the scientific foundation for future ArM technology that can impart selectivity to high value chemical reactions, including C-H bond functionalization and olefin polymerization, *in vitro*. Such improvements in reaction control are essential for preparing advanced, well-defined materials including polymers for tissue engineering and biologically active small molecules. Long-term goals involve enabling this technology *in vivo*, where ArMs could interact with endogenous proteins and metabolites to modify the function of host organisms, ultimately humans, in a controlled fashion.

B. Action Selection under Time-Pressure

Professor Scott Grafton, University of California - Santa Barbara, Institute for Collaborative Biotechnologies (UARC)

This research focuses on acquisition and analysis of physiologic measurements of the brain and peripheral autonomic nervous system that contain features that reflect action uncertainty or choice in the face of different sources of stress. The objectives are to (1) demonstrate feasibility of pattern classification of electroencephalogram (EEG) and or functional magnetic resonance imaging (fMRI) data for detecting levels of uncertainty in simple laboratory paradigms requiring action decisions and control; (2) determine how payoff structure influences behavior in time-pressure responses; (3) develop technologies that characterize stress response based on peripheral physiologic measurements; and (4) develop tools for diffusion image analysis to characterize structural differences between individuals. The major accomplishments on this project in the past year include discovery that explicit knowledge of a skill increased vulnerability to choking, whereas implicit retrieval did not; discrimination of fMRI activities patterns between success and failure performances using a state-of-the-art multi-voxel pattern analysis technique; and that learning induces an autonomy of sensorimotor systems and that the release of cognitive control hubs in frontal and cingulate cortices predicts individual differences in the rate of learning (see FIGURE 3).

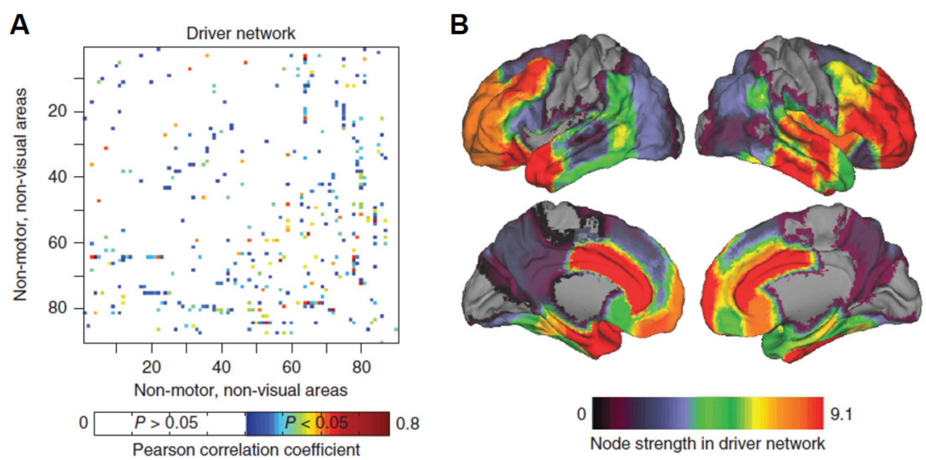

FIGURE 3

The release of a fronto-cingulate control network predicts individual differences in learning. (A) Elements in the driver network are given by the statistically significant. (P < 0.05, uncorrected) Pearson correlation between individual differences in training-induced modulation and individual differences in learning. Colors indicate the magnitude of the Pearson correlation coefficient. (B) The strength of brain areas mapped onto the cortical surface. The areas of high strength in the driver network were predominantly located in the frontal cortex, anterior cingulate and basal ganglia including the nucleus accumbens and putamen, suggesting that the training-induced release of a frontal-cingulate system predicts individual differences in learning.[2]

[2] Bassett, Yang, Wymbs, Grafton. (2015). Learning-induced autonomy of sensorimotor systems. *Nature Neuroscience.* 18:744-751.

C. Investigating the Metabolic Mechanisms of Bacterial Persistence
Professor Mark Brynildsen, Princeton University, Single Investigator Award

Within a bacterial culture, there exists a very small subpopulation of persistent cells that are viably maintained in the presence of antibiotics. Persisters are not genetic mutants, but rather phenotypic variants that temporarily cease to replicate. Cells in this “shutdown” subpopulation exhibit a drastic decrease in protein synthesis but sufficient metabolism to maintain culturability. The presence of persisters becomes especially important when considering deleterious conditions such as infected wounds and contaminated food supplies as this bacterial subpopulation is recalcitrant to traditional antibiotic and antimicrobial treatments. Characterization of the active metabolic pathways in persisters can provide new approaches toward eradication of this subpopulation. However, the presence of only a very low percentage of persister cells within a culture presents a significant challenge in attempts to isolate persisters and characterize their metabolic programming.

Professor Brynildsen has engineered a means to address this challenge and has provided an initial understanding of some of the key metabolic features of bacterial cells as they enter the persistent state. Brynildsen takes advantage of the observation that the terminal effectors of the transition from normal physiology to persistence are encoded by a number of toxin-antitoxin modules present in the bacterial genome and that entry into persistence is driven in the rare instances where free toxin accumulates in the cell. Professor Byrnildsen has constructed *E. coli* strains that allow for orthogonal expression of toxins and antitoxins providing a controlled means of inducing, maintaining and shutting down the persister state in an entire bulk culture (see FIGURE 4).

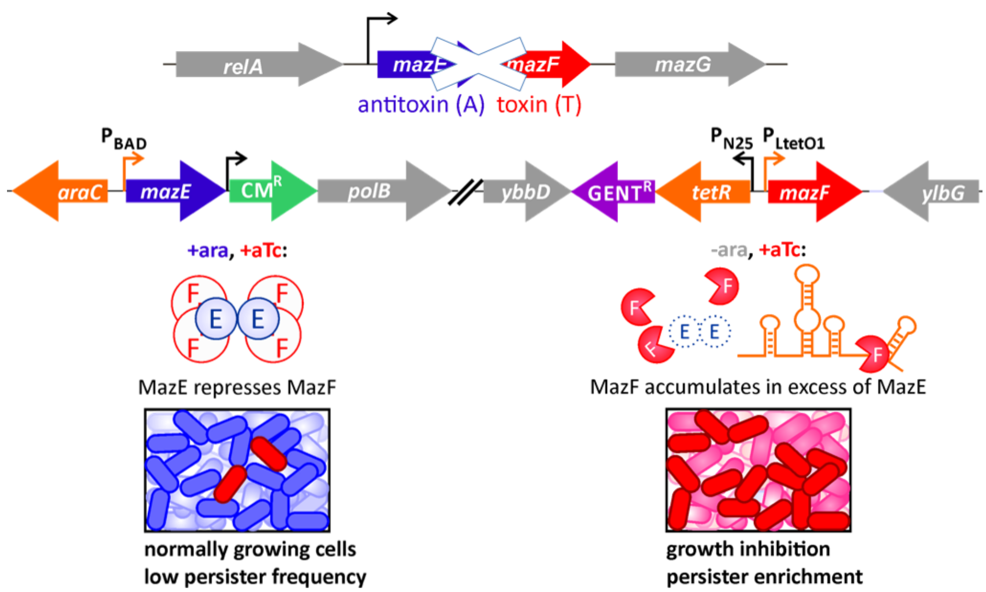

FIGURE 4

Genetic construction for orthogonal toxin/antitoxin induction. In an *E. coli* strain with the native mazE and mazF antitoxin/toxin genes deleted, genetic constructs are designed for arabinose-induced expression of the mazE-encoded antitoxin and the tetracycline-induced expression of the of the mazF-encoded toxin. With both genes expressed, MazE and MazF forms a high affinity complex that represses the MazF toxin activity. With induction tuned so that MazF accumulates in excess of MazE, free MazF toxin accumulates leading to an enriched persistence state in the bulk culture.

Following preferential induction of the mazF-encoded toxin it was first demonstrated that this engineered control system does provide the means for induction of a model persister culture in that the Maz-F arrested populations were tolerant to two classes of antibiotics (β-lactams and fluoroquinones). Further it was noticed that MazF-arrested cells continue to consume oxygen and glucose at rates comparable to non-induced cells despite their limited ability to produce biomass. This inefficient use of resources led to a hypothesis that the cells are undergoing futile cycling of available nutrients. This hypothesis was supported by results from a metabolomics analysis indicating that, compared to a control culture, MazF-accumulated cells showed a significantly greater abundance of lower energy ribonucleotide mono- and di-phosphates vs higher energy ribonucleotide triphosphates (rNTPs). As MazF is an endoribonuclease, it was further postulated that MazF-arrested cells degraded newly formed transcripts furthering the idea of a futile metabolic cycle. By treating MazF-arrested cells with rifampicin, an inhibitor of RNA polymerase (RNAP), it was shown that oxygen and glucose consumption decreased significantly. Interestingly, transcriptional arrest in Maz-F arrested cells resulted in an increase in the accumulation of recharged of rNTPs compared to their mono- and di-phosphate counterparts. These results from the rifampicin-treated cultures provide support that MazF-arrested cells are undergoing a macromolecular futile cycle driven by RNAP and the endonuclease activity of MazF.

Other pathways that are indicative of the entry into persistence will be likewise characterized. Similar analyses will be performed during the stasis and exiting stages of persistence with the MazEF induced system as well as with other induced toxin-antitoxin bacterial systems that arrest growth through different mechanisms.

D. Testing a Mathematical Model of Status Processes and Faction Sizes

Professor David Melamed, University of South Carolina, STIR Award

While it is no secret that higher status actors tend to dominate groups, understanding the conditions under which their power is undermined and their influence falters is not well understood. Professor Melamed developed a new mathematical model of the relationship between status and influence by taking into account how status is distributed in social groups. In this approach, status distributions trigger psychological processes that make members more or less amenable to social influence. In particular, Professor Melamed proposes that status distributions can create competing factions in groups that reduce perceptions of uncertainty among faction members regarding a course of action. This uncertainty reduction, in turn, makes members more resistant to external attempts at influence and more cohesive as a group (see FIGURE 5). As a result, they are (i) less likely to conform to influence attempts from higher status group members; and (ii) more likely to press high status group members to conform to their own positions. Previous research has not been able to explain sudden shifts in the influence levels of high status group members and their fall from power in groups. Most commonly, scientists have assumed that leadership (i.e., high status) failures were a function of either aid from external high status actors to the low status group members attempting to overthrow leaders or leader mortality (without a succession plan). Cases in which low status group members suddenly seized power were unexplained and often considered an anomaly until this model was developed.

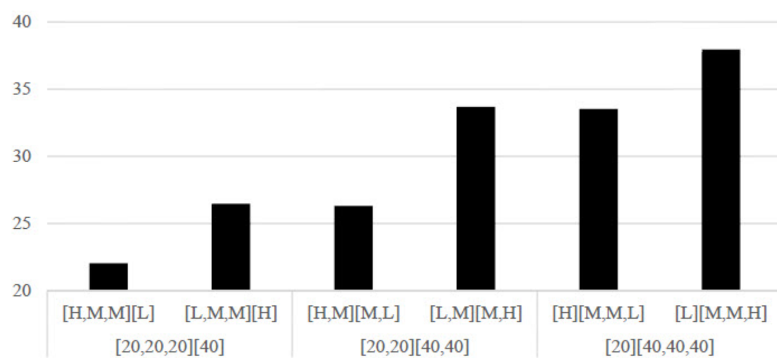

FIGURE 5

Status Faction Theory. The bars indicate predicted group decisions given the relative status of members (H = High Status, M = Medium Status, L = Low Status) and initial opinions of members, in brackets below status distributions, ranging from 20 – 40. As the bar graph shows, high status actors' influence over group members declines as medium and low status actors coalesce around a common position.

Professor Melamed's experiments confirmed the model predictions, providing striking new insight on the dynamics through which influential individuals can be undermined. In these experiments, as the number of low status group members increased vis-à-vis the number of high status actors, the influence rates of higher status group members declined and uncertainty among the low status actors regarding their position decreased. Professor Melamed also noted a proportional increase in uncertainty of high status actors as the proportion of low status actors increased, which led to decays in their response time. A key contribution of this work is that it demonstrates both the social structural (i.e., status distributions) and psychological mechanisms (i.e., uncertainty reduction) at play when group members are vying to take control of a collective. Combined, these mechanisms represent a powerful channel that can lead to the toppling of leaders, the expression of minority opinions, and the rise of previously weak factions within a society.

E. Modeling the Dynamics of Conflict and Cooperation within and between Multifarious Social Groups

Professor Sergey Gavrilets, University of Tennessee, Single Investigator Award

Under what conditions to individuals risk their own resources and lives to contribute to a group? Addressing this question has been an ongoing challenge in the social sciences. Collective resources, such as food and water, are essential to the survival of social organisms, and once acquired, must be managed by the group and protected from attempts of other groups to seize them. Yet, there is often an incentive for individual group members to "free-ride" (i.e., reduce or eliminate any contribution of support, while still benefiting from the public good that others are supporting). If all group members take a free-ride, however, the survival of the group is put at risk. Conventional research has long assumed that the fewer free-riders there are in a group the greater the group's likelihood of survival. Furthermore, existing theories suggest that free-riding is most likely when groups face the greatest threats. Thus the solution the free-rider problem is to ensure adequate costs for free-riding are imposed and incentives for contributions are offered, particularly when competition from other groups is keen. This creates an inefficient and costly system, however. This year, Professor Gavrilets, demonstrated the viability of a new evolutionary model of cooperation emerging from conflict with competing groups to address the free-rider problem. Professor Gavrilets' research successfully demonstrated that in groups facing competition from other collectives, if individuals contribute to the protection of resources from raids by external groups, they develop improved ability to cooperate and secure more resources even when competition is absent. This, in turn improves the fitness of the group and may even improve social intelligence, ongoing social evolution, and the capacity of the group to thwart attempts of other groups to seize their resources (see FIGURE 6).

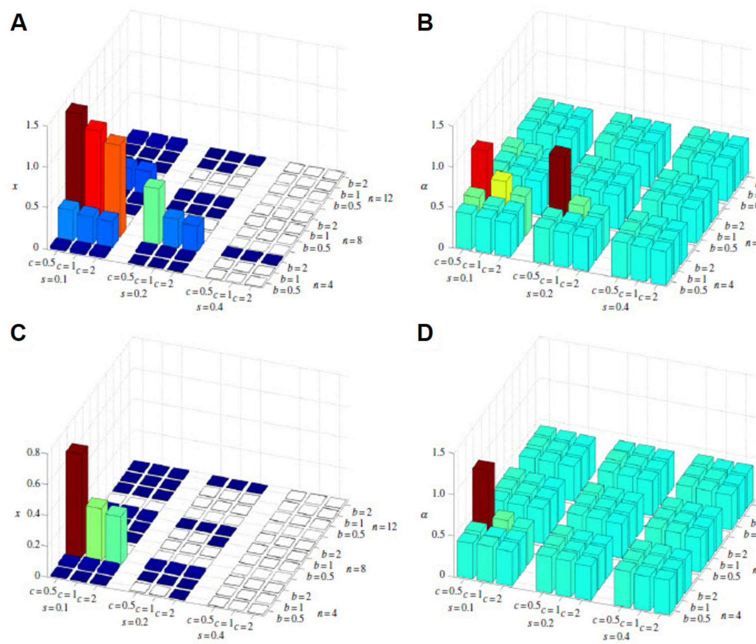

FIGURE 6

Efforts contributed to protect collective resources. Each panel shows the effects of four parameters (benefit of collaboration, b, cost of individual effort, c, cost of collaboration, s, and group size, n) on average equilibrium values for individual effort (graphs (A) and (C)) and collaborative ability (graphs (B) and (D)). When individual effort emerges in the face of conflict (A), collaborative efforts in the absence of conflict are higher (B), in comparison to individual effort expended in the absence of conflict (C) and subsequent collaboration in the absence of conflict (C).

The model suggests the importance of social structure in determining the optimal distribution of costs and benefits to discourage free-riding. Unexpectedly, it also shows that when collaboration emerges in competitive situations, the collaboration continues, rather than decaying as in traditional rational models focusing purely on cost-benefit structures. In FY16, Professor Gavrilets will conduct a series of experiments to test these models among human groups in the U.S. and U.K. He will examine how and under what conditions competitive environments generate increased propensity for collaboration and the extent to which those collaborative tendencies persist in the absence of competition.

F. Dynamic Network Neuroscience

Professor Danielle Bassett, University of Pennsylvania, Single Investigator Award

Cognitive processes that harness distributed networks of brain areas drive human behavior. For decades, the focus was to pinpoint brain region(s) associated with behavior. Emerging work shows this approach is flawed; the mammalian brain is constantly reconfiguring the relative connections among brain regions to enable learning, memory, and cognition. Rather than a static snapshot of brain function that may apply broadly to the population, it is clear that brain communication patterns are dynamic and are not necessarily stereotyped across individuals. The reconfiguration of brain activity and connectivity is particularly relevant to mission outcomes in the context of neural (and by extension behavioral) adaptation. Adaptation can be broadly defined as any alteration in the structure or function of an organism or any of its parts by which the organism becomes better fitted to survive and succeed in its environment. Long-term adaptation is a hallmark of learning, and therefore a common goal of training. Shorter time-scale adaptations are particularly salient for operational consideration in the form of cognitive flexibility to efficiently change a cognitive state or the ability to shift a decision criteria based on new and incoming information. These and related forms of adaptation enable a warrior to optimize his/her response to training, complex scenarios on the battle field, and rehabilitation following physical or psychological injury. Neural adaptation also plays a key role in soldier interactions with machine and computer interfaces, informing the use of these interfaces in combat and performance enhancement. An understanding of these processes in large-scale brain circuitry has been hampered by the current lack of any approach to quantify, characterize, or predict these processes from non-invasive neuroimaging data in humans.

In FY15 a robust set of analytical tools was established from applied mathematics to treat the patterns of communication between brain regions as evolving networks whose reconfiguration dynamics are tightly linked to performance. This method allowed Professor Bassett and colleagues to quantify the network dynamics related to structural and functional communication over short and long time scales and predict the adaptation of neural circuits measured non-invasively in individual human subjects. The general approach began with a functional magnetic resonance imaging (fMRI) scan acquired from a single human participant during learning of motor tasks over the course of 6 weeks. Professor Bassett's work is providing a cohesive and statistically-principled account of the dynamics of distributed and integrated neural circuits during cognitive processes in behaving humans (see FIGURE 7). This research facilitates important opportunities for studying the cognitive neuroscience of learning and could lead to the development of new theories about the relationship of cognitive processing to performance. This foundational knowledge enables new approaches for training expert learning and performance faster and more efficiently based on the functional dynamics of the individual's brain.

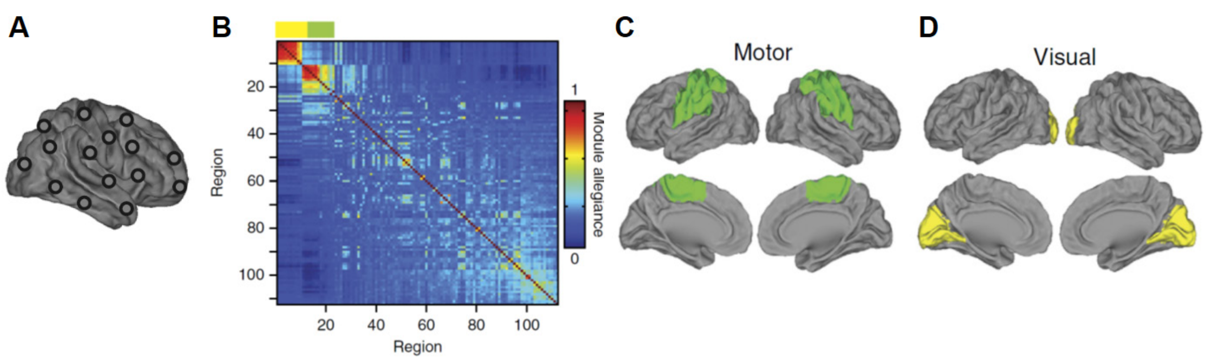

FIGURE 7

Recruitment and allegiance across brain regions. (**A**) To address the question of whether there are sets of brain regions that preferentially interact during task performance brain scan images were parcellated into 112 cortical and subcortical regions. (**B**) Functional connectivity was calculated across these regions as human subjects performed a motor skill learning task. The probability of communication was calculated between any two regions and quantified as an allegiance statistic for that pair. Within each row/column of the module allegiance matrix, the average allegiance value within a system yields the recruitment coefficient. (**C**-**D**) Two sets of functional modules emerged from these analyses. One set (C) was composed of primary and secondary sensorimotor regions and the other (D) composed of primary visual cortex. These two regions were consistently grouped into the same network community. This suggests that brain areas relevant for task execution are functionally coherent throughout learning whereas the other areas important for cognition are only transiently coherent.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Virus Directed Assembly of Peptide Receptor Surfaces

Investigator: Professors Jim Culver and Reza Ghodssi, University of Maryland, Single Investigator Award
Recipient: ARL-SEDD

Biologically derived peptides offer a unique source of recognition specificity for the detection and identification of a range of threats including explosives, toxins and viruses. However, incorporation of these peptides into robust sensor systems has been challenging due to a gap in our abilities to assemble and integrate these selective peptides into sensor devices. To address this challenge, this research effort is focused on utilizing the rod-shaped macromolecular structure of the Tobacco mosaic virus (TMV) as a nano-platform to control the display, assembly and integration of receptor peptides onto sensitive transducer surfaces.

As part of this effort, the research team developed an *E. coli* expression system for production of TMV virus-like particles (VLPs) to circumvent challenges faced when replication of active TMV virus particles resulted in loss of displayed peptides due to recombination. The TMV VLPs are the first VLPs to self-assemble within *E. coli* and are highly stable, enabling the incorporation of receptor peptides in multiple configurations on the surface and of the rod-shaped particles. The team also created variants of the TMV VLPs that permit the display of receptor peptides within the inner channel of the rod-shaped VLP in addition to the outer surface. One of these variants additionally increased the diameter of the inner channel from 4 nm to 8 nm by genetically removing a loop from the VLP subunit. As an initial test of the TMV VLP scaffold, a peptide that binds TNT was incorporated onto the surface of the VLP, and specific binding of TNT by the modified VLP was detected.

The TMV VLP platform has the potential to serve as a universal scaffold for the presentation of diverse receptor peptides. Scientists at ARL-SEDD have followed this research since its inception, due to interests in peptides as recognition elements. Independent research conducted by ARL-SEDD developed a novel approach to isolate receptor peptides with specificity for a given target. As proof of concept, this methodology was used to identify a novel receptor peptide that binds aluminum. As a collaborative effort, this peptide sequence was provided to the research team at the University of Maryland, and this peptide was successfully incorporated into a TMV VLP. This construct will be evaluated by the research team at the University of Maryland and ARL-SEDD to determine if the TMV VLP scaffold may facilitate the incorporation of ARL-generated peptide reagents into sensor systems.

B. Rapid Diagnostic Tool for Wound Infections

Investigator: Dr. Ravi Verma, Spectral Platforms, Inc., SBIR Phase II Award
Recipient: Dr. Tyler Bennett, US Army Medical Materiel Agency (USAMMA)

Spectral Platforms, Inc. has used Army SBIR Phase II support to develop and validate a rapid diagnostic solution for the detection and characterization of any pathogenic microorganism in blood/urine/CSF. The solution is based on a new biomarker that they have developed comprising lycopene incorporated into human serum albumin. When pathogenic microorganisms are present, the albumin binds to the microorganism, and aggregates lycopene on the bacteria surface. This alters the optical signature of the lycopene, even for clinically relevant pathogen concentrations, and these optical changes can be detected with low cost optical instrumentation. With the SBIR support, the company has developed this new technology, validated it with 250 patient samples, and also had it externally validated at the Freeman Hospital in the UK with artificially inoculated samples. The instrumentation developed under this award rapidly (within 15 minutes) characterizes the presence or absence of any pathogenic microorganism in blood and characterizes the response of that microorganism to a candidate antimicrobial.

The ARO Life Sciences and Electronics Division recently selected Spectral Platforms for a Phase II enhancement contract from the Army SBIR office to further develop the technology with matching funds from the US Army Medical Materiel Agency (USAMMA). Under this Phase II enhancement award, Spectral Platforms will (a) develop a quality system to ensure that the products and reagents used conform to the required tolerances, (b) develop a technical file documenting all of the critical parameters related to the performance and implementation of the system, (c) prepare a determination pre-Investigational Device Exemption (pre-IDE) submission for the FDA including details of a proposed clinical study protocol for device validation, (d) perform an extensive clinical validation study, (e) compile the results of the clinical study and submit 510K filing to the FDA for approval.

USAMMA views the Spectral Platforms systems as an intriguing medical device technology and of sufficient Technology Readiness Level to move into advanced development toward its approval for use by the US FDA. As a co-funder and transition partner for this technology, USAMMA will work with Spectral Platforms to assess the utility of the technology as applied to pathogens of interest to the USAMMA. USAMMA is also willing to provide their own expertise and assistance in gaining access to facilities and materiel necessary for this effort to succeed. If the technology can successfully demonstrate the required capabilities, it will be a candidate for further development at USAMMA.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Engineering Nanoscale Protein Containers

Professor Danielle Tullman-Ercek, University of California - Berkeley, Single Investigator Award

Polyhedral protein-based microcompartments are ~125 nm enclosed scaffolds that natively encapsulate enzyme pathways in bacteria, and are promising structures for the bacterial production of chemicals and pharmaceuticals (see FIGURE 8). They hold great potential for future applications, including in vitro nano-containers and drug delivery devices, due to the precise structure and size of these protein assemblies. Segregating reactions in such compartments offers multiple potential advantages: (i) sequestration of toxic or highly reactive substrates or intermediates; (ii) enhanced kinetics for product synthesis; (iii) creation of unique interior environments; and (iv) avoidance of off-pathway competing reactions. Recently, encapsulation of a synthetic, two-enzyme ethanol production pathway in a microcompartment resulted in higher yields compared to an unencapsulated pathway *in vivo*. This result opens the door for additional pathways to be compartmentalized, but hurdles remain before this technique can be widely applied either within the cell or in other contexts. It is not known how to adjust the number, size, shape, and cargo loading of microcompartments, and the ability to tune these parameters will be essential for optimal performance. For example, yields are expected to correlate with the number of microcompartments per cell, yet there are no known mechanisms for altering the microcompartment concentration, and any imbalance in protein shell components leads to misformed structures or aggregation. Moreover, enzyme targeting to interior of the microcompartment is only understood for single enzymes; competition between multiple enzymes and control over stoichiometry is as yet unexplored. Finally, the rules governing assembly and cargo encapsulation *in vitro* are unresolved.

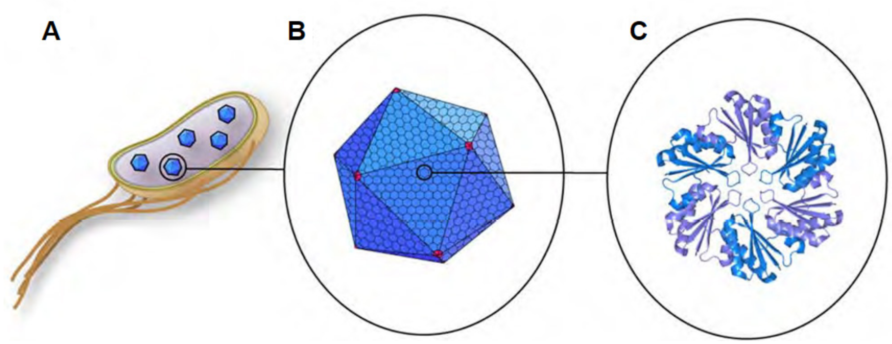

FIGURE 8

Bacterial microcompartments. (A) These bacterial structures compartmentalize enzyme reactions in cells. (B) The structures are polyhedral and consist of multiple constituent proteins that form vertices (red) and facets (blue). (C) The facets consist of hexamers of a single shell protein.

To advance the translation of these scaffolds to applications for synthetic biology and beyond, Prof. Danielle Tullman-Ercek at the University of California - Berkeley is developing a detailed fundamental understanding of microcompartment regulation and assembly, as well as exploring approaches to precisely control the amount and stoichiometry of enzymes loaded within these structures. It is anticipated that in FY16, ribosome binding site engineering will be completed to optimize shell protein expression and assembly into microcompartments *in vivo*. In addition, the eight known shell-forming proteins for the propanediol utilization (Pdu) microcompartment will be purified and a pull-down assay will be established to probe shell protein interactions.

This will enable a combinatorial exploration of the structures that form when shell-forming proteins are combined in different concentrations and ratios.

Protein-based containers could advance technologies supporting several new Army and DoD capabilities, including production of specialty chemicals, drug delivery and nanomaterial fabrication. When used in bacteria, engineered microcompartments could facilitate biological production of previously incompatible chemicals. Beyond the cellular environment, this research could lead to creation of "organelles" within artificial cells, offering spatial sequestration of components as needed for the design of these systems. Artificial cells hold promise for further expanding the set of conditions at which biological syntheses can be performed to produce specialty chemicals or materials. The research will also inform the controlled assembly of protein-based nanoscale structures. Such assemblies could be used as nanoscale bioreactors, which could carry out enzymatic reactions in non-aqueous solvents to enable production of polymers, explosives, and other chemicals that normally require tremendous infrastructure to produce synthetically.

B. The Neurodynamics of Social Status

Professor Will Kalkhoff, Kent State University, Single Investigator Award

An ongoing challenge for the social sciences is understanding the relationship between social structure, biophysiological states, and social behavior. Professor Kalkhoff is taking on this challenge by testing a new theory that relates social dynamics to neurological states. This research posits that two social dynamics can be measured by distinct neural activity as measured through electroencephalogram (EEG) and functional magnetic resonance imaging (fMRI): (1) threats to one's identity posed by the challenges another makes to one's identity; and (2) unexpected behaviors of others with whom one is collaborating. Professor Kalkhoff advances status influence theory by treating status as a form of identity, which when threatened, creates a sense of identity loss that is related to a change in neural activity (see FIGURE 9). Also, however, Professor Kalkhoff proposes that when status is not threatened or even subject to elevation, the shift in neural activity is much more sublime. Both threats and elevation, however, correspond to unexpected events, which Professor Kalkhoff hypothesizes are detected through different changes in neural activity.

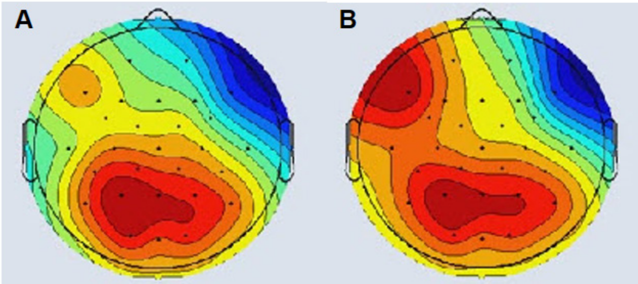

FIGURE 9

Neural activity under identity threat. (A) Neural activity, as captured via electroencephalogram (EEG) output, during problem-solving in a non-threat situation. Orange and red regions indicate areas of greater activity, while blues and green hues indicate regions of less activity. (B) Shifts in activity as measured through EEG when an individual's identity is threatened. The shift occurs approximately 200-300 milliseconds after the unfavorable identity threat event occurs.

In addition, Professor Kalkhoff is examining how fMRI and EEG patterns across two actors converge as they collaborate to solve a problem in the absence of unexpected violations of status hierarchies. This element of the research suggests that cohesiveness can also be detected by examining synchronicity across group members in brain activity. As the theory and methodology are tested in the coming year, Professor Kalkahoff's research has the potential to break new ground in understanding the neural dynamics of social interaction, influence, and deviance, as well as developing new methods to detect the degree of cohesiveness in groups.

C. Computational Models of Cultural Meaning and Social Interaction

Professor Dawn Robinson, University of Georgia, Single Investigator Award

An understanding of local cultures is increasingly important for decision-making on a global stage and achieving cultural competence across the many venues in which military operations are carried out remains difficult. Theoretical models that can be generalized across cultures have been difficult to achieve, but Professor Robinson's research is providing a compelling new approach, by developing new advances in Affect Control Theory (ACT), a mathematical model of cultural meaning, which is proving adaptable to any culture. The uniqueness in ACT's theoretical strategy is its reliance on linguistic distinctions to capture culture. Yet, assessing culture through ACT does not require that one be an expert in the linguistics of a cultural group. Instead, the approach creates mathematical models of meaning. Professor Robinson's research entails developing new Bayesian models to capture cultural meaning. Already, Professor Robinson has demonstrated that the models are capturing unique differences between such diverse cultures as Canada, Japan, Germany, China, Kuwait, and Egypt (see FIGURE 10).

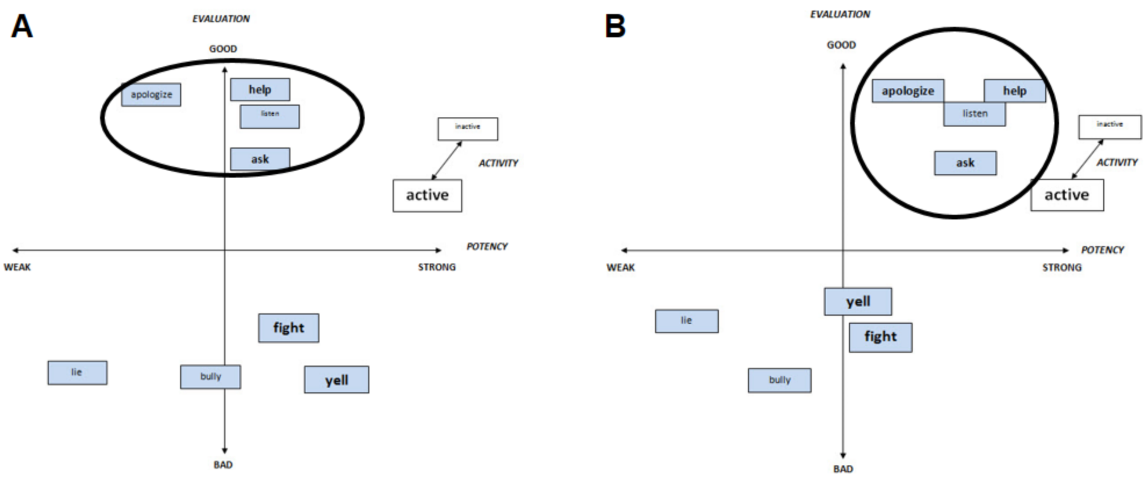

FIGURE 10

Differences in three dimensions of cultural meaning across US and Arabic cultures. Behaviors perceived as "good" in US culture are also somewhat neutral when it comes to perceptions of power. In panel (**A**) for US culture, these behaviors (circled) are high on the good-bad vertical axis, but toward the middle in the weak-strong potency horizontal axis in panel (**A**). Note, however, that the same circled behaviors are similarly high on the good-bad vertical axis for Arabic cultures, noted in panel (**B**). Yet, they are perceived as more powerful in the Arabic culture vis-à-vis US culture, as indicated by their relative position on the horizontal potency axis.

These models if cultural meaning are parsimonious, relying on just three dimensions (power, morality, and activity) that underscore the overall meaning of actors and their behaviors in social interaction. Importantly, these three dimensions can capture subtle cross-cultural nuances in meaning. Furthermore, Professor Robinson's models are not only are able to capture the meaning of a particular behavior at a particular point in time; they can also predict (a) responses of observers of the behavior; and (b) subsequent adjustments by the actor exhibiting the behavior. Consequently, this research represents a promising theoretical approach has the capacity for simulating dynamic chains of behavior, enabling the capacity to predict within- and cross-cultural interaction without relying on deep cultural expertise. In the coming year, Professor Robinson will continue to refine the mathematical representation of the model and test it on additional cultures.

D. Multi-scale Dynamics of Cortical Adaptation for Human Auditory Detection

Professor Dana Boatman, Johns Hopkins University, Single Investigator Award

The ability to detect and respond rapidly to novel sounds is critical for survival. Animal electrophysiology studies have shown that short-term cortical adaptation facilitates detection of novel sounds even when not actively attending to the environment. Adaptation refers to reduced neural activity for repeated or ongoing (background) sounds and is a form of experience-dependent cortical plasticity. However, the temporal properties of adaptation in human cortex are poorly understood. Specifically, it is not known whether adaptation occurs during early stages of sound detection, or reflects higher-level cortical processes. The dearth of high resolution human data, coupled with morphological differences between human and animal auditory cortex, has hampered efforts to develop realistic computational models of cortical auditory processing. Computational neural network models of sensory processing have focused mainly on visual cortex and have been largely unexplored in auditory cortex. Moreover, development of neural network models is rarely based on in vivo data, leading to potentially unrealistic representations of sensory processing. This project attempts to address both shortcomings by developing a realistic neural network model of auditory cortex based on human intracranial recordings. Professor Boatman's research will provide fundamental understanding of early auditory processing in human cortex and how it is modulated by stimulus statistics and attention.

In FY16, Professor Boatman and colleagues will tune a multi-compartmental neocortical model to simulate short-term adaptation of local cortical activity, including firing patterns. The model will be used to analyze data from human electrocorticography recordings during active listening in awake human subjects (see FIGURE 11). The model will be used to test three proposed mechanisms of adaptation: gain control, neural sharpening and top-down facilitation. This research may enable a realistic biophysical model of neural network dynamics associated with real-world listening conditions that include degraded, competing and multimodal (auditory-visual) inputs, as well as fluctuations in listener state (attention, fatigue). Understanding the temporal dynamics of adaptation in human cortex will be important for improving detection of novel sounds, including speech, in real-world listening environments.

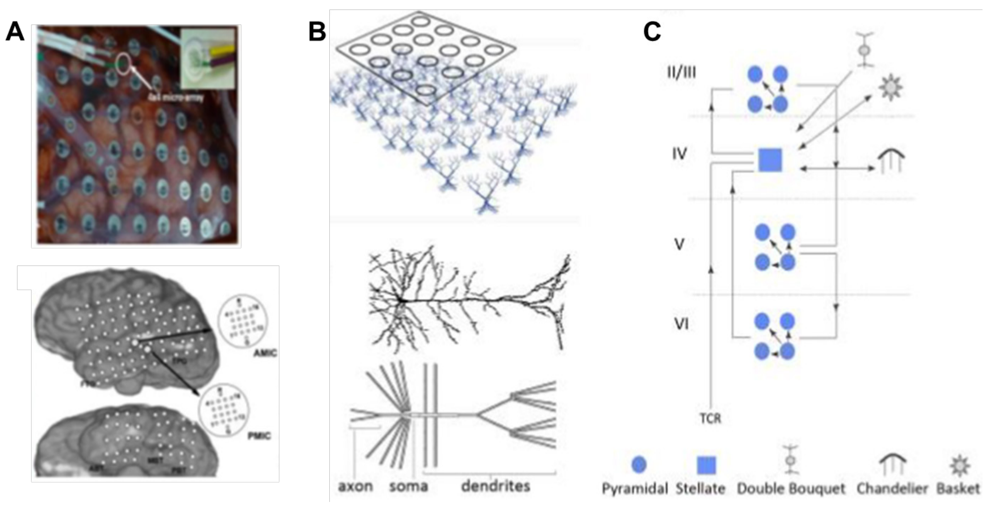

FIGURE 11

Human electrocorticography and neocortical modeling. (**A**) Intra-operative photo of macro- and micro-electrocorticography grid array placement. Bottom, left hemisphere lateral and mesial 3D MRI reconstruction showing implanted arrays and coverage of superior temporal gyrus. (**B**) Schematic of Layer II/III neuronal network in modeled minicolumn with modeled micro-elements above to represent 4x4 micro-electrode recording array on cortical surface. Note: inter-cell and inter-electrode distances are rescaled for visualization; actual scale factor ratio is approximately 50:1. Bottom, in vivo pyramidal cell (top) and modeled pyramidal cell (bottom). (**C**) Diagram of cellular architecture and connectivity in modeled minicolumn. Omitted for visibility are: Layer IV pyramidal cells, Layer I containing pyramidal apical dendrites from Layers II/III; inhibitory connections to other layers, and thalamic reticular nucleus input.

E. Metabolic Activities in Dormant Spores

Professor Peter Setlow, University of Connecticut, Single Investigator Award

Bacteria of *Bacillus* species can grow vegetatively if conditions such as nutrient availability and other environmental conditions are appropriate. However, if conditions in media become inappropriate for growth, such as reduced nutrient availability, *Bacillus* can initiate a genetic program called sporulation. During sporulation, the spore becomes dormant taking on a number of novel layers in its outer regions and physical changes to the inner membrane and central core. This change in morphology renders the cell extremely resistant to all manners of environmental insults including heat, desiccation, radiation and toxic chemicals. Because of their dormancy and extreme resistance, spores of many species can persist in environments for many years and are the vectors for foodborne spoilage and food borne diseases. It has long been accepted that spores have no metabolic activity. However, this dogma has been called into question by a 2012 paper published by the laboratory of Sigal Ben-Yahuda of the Hebrew University of Jerusalem that provided evidence that there was massive rRNA and mRNA degradation as well as significant transcription in dormant *Bacillus subtilis* spores held at 37 or 50ºC for 3-8 days.

The Setlow laboratory followed up this work and found evidence of slow metabolic activity of spores stored at these temperatures, but only in spent sporulation medium, not during storage in water and no ATP was detected. The Setlow lab was recently funded through the ARO Single Investigator Program to rigorously extend these initial studies to establish the magnitude of this metabolism and its effects on dormant spore properties. In FY16, the Setlow group will use ^{13}C- and ^{31}P-NMR and various enzymatic assays to identify and quantify low molecular weight catabolites in spores as well as the fate of new catabolites during dormancy using B. subtilis variants that lack all nutrient germinant receptors (GR's). Use of these variants are a suitable safeguard against the presence of any "leaky" germination that can complicate the interpretation of results. Likewise, GR-less *B. subtilis* will be used to assess the level of rRNA degradation and to start examining synthesis and degradation of specific mRNAs at different sporulation conditions. These rigorous approaches will provide new insights on what "dormancy" actually means within the context of how bacterial spores prepare for dormancy, act during dormancy and whether metabolic changes during dormancy alter spore properties.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Micheline Strand
Division Chief
Program Manager, Genetics

Dr. Stephanie McElhinny
Program Manager, Biochemistry

Dr. Frederick Gregory
Program Manager, Neurophysiology and Cognitive Neuroscience

Dr. Robert Kokoska
Program Manager, Microbiology

Dr. Lisa Troyer
Program Manager, Social and Behavioral Science

B. Directorate Scientists

Dr. Douglas Kiserow
Director, Physical Sciences Directorate

Dr. Peter Reynolds
Senior Scientist, Physical Sciences Directorate

Dr. J. Aura Gimm
Program Manager, Institute for Soldier Nanotechnologies and Institute for Collaborative Biotechnologies

Dr. Kelby Kizer
Special Assistant to the Directorate Director

Dr. Larry Russell, Jr.
International Research Program Coordinator

Mr. John McConville
Technology Transfer Officer, Institute for Soldier Nanotechnologies

C. Administrative Staff

Ms. Wanda Lawrence
Contract Support

CHAPTER 7: MATERIALS SCIENCE DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2015* is to provide information on the programs and basic research supported by ARO in fiscal year 2015 (FY15), and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Materials Science Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY15.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Materials Science Division seeks to realize improved material properties by embracing long-term, high risk, high-payoff opportunities for the U.S. Army, with special emphasis on four Program Areas: Materials by Design, Mechanical Behavior of Materials, Physical Properties of Materials, and Synthesis and Processing of Materials. The objective of research supported by the Materials Science Division is to discover the fundamental relationships that link chemical composition, microstructure, and processing history with the resultant material properties and behavior. These research areas involve the discovery of the fundamental processes and structures found in nature, as well as developing new materials, material processes, and properties that promise to significantly improve the performance, increase the reliability, or reduce the cost of future Army systems. Fundamental research that lays the foundation for the design and manufacture of multicomponent systems such as composites, hierarchical materials and "smart materials" is of particular interest. Other areas of interest include new approaches for materials processing, composite formulations, and surface treatments that minimize environmental impact. Finally, there is general interest by the Division in research to identify and fund basic research in manufacturing science, which will address fundamental issues related to the reliability and cost (including environmental) associated with the production and long-term operation of Army systems.

2. Potential Applications. Research managed by the Materials Science Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter and battle systems. In the long term, the basic research discoveries made by ARO-supported materials research is expected to provide a broad base of disruptive and paradigm-shifting capabilities to address Army needs. Advanced materials will improve mobility, armaments, communications, personnel protection, and logistics support in the future. New materials will target previously identified Army needs for stronger, lightweight, durable, reliable, and less expensive materials and will provide the basis for future Army systems and devices. Breakthroughs will come as the fundamental understanding necessary to achieve multi-scale design of materials, control and engineering of defects, and integration of materials are developed.

3. Coordination with Other Divisions and Agencies. To realize the vision of the Materials Science Division and maximize transition and leveraging of new materials discoveries worldwide, the Division collaborates with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the Defense Advanced Research Projects Agency (DARPA), and across federal-funding agencies (*e.g.*, Nanoscale Science and Engineering Technology subcommittee, Reliance 21 Community of Interest for Materials and Processes), and in international forums (*e.g.*, the Technical Cooperation Program). The Materials Science Division is also very active in collaborating with other ARO Divisions to co-fund research, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. In particular, ongoing collaborations exist with the ARO Chemical Sciences, Electronics, Life Sciences, Mechanical Sciences, Mathematical Sciences, and Physics Divisions.

B. Program Areas

The Materials Science Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY15, the Division managed research within these five Program Areas: (i) Materials by Design, (ii) Mechanical Behavior of Materials, (iii) Physical Properties of Materials, (iv) Synthesis and Processing, and (v) Earth Materials and Processes. As described in this section and the Division's BAA, these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Materials by Design. The Materials by Design Program Area seeks to establish the experimental techniques and theoretical foundations needed to facilitate the hierarchical design and bottom-up assembly of multifunctional materials that will enable the implementation of advanced materials concepts including transformational optics, biomimetics and smart materials. This Program Area is divided into two research Thrusts:

(i) Directed 3D Self-Assembly of Materials is aimed at enabling the directed 3D assembly of reconfigurable materials, and developing viable approaches to the design and synthesis of multi-component materials incorporating hierarchical constructs.

(ii) Functional Integration of Materials focuses on demonstrating the predictive design and integration of functional properties into complex multi-component systems, and developing analytical techniques for interrogating the evolution of the 3D structure and properties of material assemblies at the nanoscale.

2. Mechanical Behavior of Materials. The Mechanical Behavior of Materials Program Area seeks to reveal underlying design principles and exploit emerging force-activated phenomena in a wide range of advanced materials to demonstrate unprecedented mechanical properties and complementary behaviors. This Program Area is divided into two research Thrusts:

(i) Force-Activated Materials involves demonstration and characterization of robust mechanochemically adaptive materials based on force-activated molecules and force-activated reactions, tailoring the deformation and failure mechanisms in materials to mitigate the propagation of intense stress-waves and control energy dissipation, and the creation of a new class of adaptive structural materials that demonstrate "mechanical homeostasis."

(ii) Mechanical Complements in Materials discovers superior ionic transport materials and transparent materials through a complementary, interdependent, optimization of mechanical properties, catalyzes a self-sustaining investigation of fiber precursors, tailored for lateral and axial interactions, to generate new paradigms for revolutionary structural fibers, and discovers and validates new atomic-scale strengthening mechanisms governing bulk mechanical behavior.

3. Physical Properties of Materials. The Physical Properties of Materials Program Area seeks to elucidate fundamental mechanisms responsible for achieving extraordinary electronic, photonic, magnetic and thermal properties in advanced materials to enable future Army relevant innovations. This Program Area is divided into two research Thrusts:

(i) Free-standing 2D Materials focuses on the creation of novel free-standing 2D materials, heterostructures and hybrids with physical properties complementary or superior to graphene, and the invention of novel characterization techniques specific to 2D materials to determine unprecedented properties.

(ii) Defect Science & Engineering explores the specific influence of defects (positive or negative) on the physical properties of novel functional materials, and elucidates defect control mechanisms during thin film growth and bulk processing of novel functional materials.

4. Synthesis and Processing of Materials. The Synthesis and Processing of Materials Program Area seeks to discover and illuminate the governing processing-microstructure-property relationships for optimal creation of superior structural and bulk nanostructured materials. This Program Area is divided into two research Thrusts:

(i) Stability of Nanostructured Materials focuses on the creation of thermally-stable, ultrahigh strength nano-crystalline materials through interfacial grain boundary engineering, and the realization of high strength, stable nanostructured alloys via pinning nano-precipitates and internal coherent boundaries.

(ii) Manufacturing Process Science supports discovery of the fundamental physical laws and phenomena of materials processes, and the exploitation of unique phenomena that occur under metastable and complex processing conditions for the creation of revolutionary materials.

5. Earth Materials and Processes. The Earth Materials and Processes Program Area seeks to elucidate the properties of natural and man-made Earth surfaces, with the goals of revealing their histories and governing dynamics and developing theory that describes physical processes responsible for shaping their features. This Program Area is closely coordinated with the Environmental Chemistry Program Area, within the Chemical Sciences Division. This Program Area is divided into two research Thrusts:

(i) Earth Surface Materials aims to utilize experiments, models, and theory development to describe the physical and mechanical properties and behaviors of rocks, minerals, and soil, and to exploit the properties of these materials to provide quantitative information on recent and ongoing surface processes and perturbations.

(ii) Surface Energy Balance aims to determine, at Army-relevant spatial and temporal scales, how natural and artificial surfaces (e.g., soil, sand, or concrete) store and conduct energy depending on their spatial relationships, inherent material properties, and imparted features such as moisture storage and evapotranspiration.

C. Research Investment

The total funds managed by the ARO Materials Science Division for FY15 were $36.5 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY15 ARO Core (BH57) program funding allotment for this Division was $5.4 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $8.3 million to projects managed by the Division. The Division also managed $17.1 million of Defense Advanced Research Projects Agency (DARPA) programs and $0.9 million of Congressional funds. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $2.0 million for contracts. Finally, $2.8 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.3 million of ARO Core (BH57) funds, in addition to any funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY15 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY15 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY15, the Division awarded 16 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Lee Bassett, University of Pennsylvania; *Quantum Control and Engineering Defects in Boron Nitride*
- Professor Srinivasan Chandrasekar, Purdue University; *Fluid-like Flow, Surface Instabilities and Folding in Metal Plasticity and Wear*
- Professor Aditi Chattopadhyay, Arizona State University; *Multifunctional Thermoset Polymer Matrix with Self-Sensing and Self-Healing Capabilities*
- Professor Horacio Espinosa, Northwestern University Evanston Campus; *Next Generation Nano-electronics Utilizing Piezoelectricity and Piezoresistivity of 2D Materials Beyond Graphene*
- Professor Stephen Forrest, University of Michigan - Ann Arbor; *Dynamics of Charge and Energy Transport at Organic-Inorganic Semiconductor Heterojunctions*
- Professor Chunlei Guo, University of Rochester; *Study of Functional Surface Structures on Metals*
- Professor Jacob Jones, North Carolina State University; *Fluorite-Structured Oxides: A New Class of Multifunctional Materials*
- Professor Anupam Madhukar, University of Southern California; *Co-Designed Dielectric Nanoparticle Optical Metamaterial - Active Device Integrated Photonic Systems*
- Professor Yuri Mishin, George Mason University; *Stabilization and Strengthening of Nano-Crystalline Immiscible Alloys*
- Professor Evan Reed, Stanford University; *Thermodynamics and Kinetics of Phase Changes in Layered Materials*
- Professor Douglas Spearot, University of Florida - Gainesville; *Virtual Diffraction Techniques Applied to Study Dislocation-Grain Boundary Interactions*
- Professor Hariharan Srikanth, University of South Florida; *Roles of Defects and Anisotropies in Spin Caloric Properties of Complex Oxides*

- Professor Chenggang Tao, Virginia Polytechnic Institute & State University; *Fundamental Investigation of Dynamic Phenomena in Atomically Thin Layered Materials*
- Professor Andrew Wereszczak, University of Tennessee at Knoxville; *High-Pressure-Induced Structural Changes in Silicate Glasses*
- Professor Clayton Williams, University of Utah; *Single-Spin Tunneling Force Microscopy for Characterization of Paramagnetic Defects in Electronic Material*
- Professor Jinkyu Yang, University of Washington; *Woodpile Mechanical Metamaterials for Sculpting Stress Waves*

2. Short Term Innovative Research (STIR) Program. In FY15, the Division awarded six new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Micah Green, Texas Engineering Experiment Station; *Microwave Response of Carbon Nanotubes in Polymer Nanocomposite Welds*
- Professor Qizhen Li, Washington State University; *Nanostructured Mg AZ31/Ti64 Multilayer Thin Films: Mechanism of Twin-Assisted Ductility and Strength*
- Professor Joshua Robinson, Pennsylvania State University; *Nucleation, Growth, and Transformation of Novel 2D Layered Materials*
- Professor Luoyu Xu, New Mexico State University; *Mechanisms of Enhancing Impact Resistance of Layered Materials Using Thin Polymeric Interfaces*
- Professor Yongke Yan, Virginia Polytechnic Institute & State University; *Discovering High Intensity Room Temperature Vis-Spectrum Piezoluminescence in Self-Assembled Grain-Oriented Hierarchical Multilayers*
- Professor Xiaodong Yang, Missouri University of Science and Technology; *Enhancement of Light Trapping and Optical Absorption in Complex ZnO Nanostructures*

3. Young Investigator Program (YIP). In FY15, the Division awarded two new YIP projects to drive fundamental research in areas relevant to the current and future Army. The following PIs and corresponding organizations were recipients of the new-start YIP awards.

- Professor Shenqiang Ren, Temple University; *Organic Photovoltaic Multiferroics*
- Professor Nicholas Boechler, University of Washington; *Shock Mitigation With Ordered Microscale Granular Media*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY15 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *2014 Materials Research Society Fall Meeting*; Boston, MA; 30 November - 5 December 2014
- *39th International Conference on Advanced Ceramics and Composites*; Daytona Beach, FL; 25-30 January 2015
- *2015 Materials Research Society Spring Meeting*; San Francisco, CA; 6-10 April 2015
- *2015 Hypervelocity Impact Symposium*; Boulder, CO; 26-30 April 2015
- *Stress Controlled Catalysis via Engineered Nanostructures Workshop*; Providence, RI; 1-2 June 2015
- *Transducers 2015, the 18th International Conference on Solid-State Sensors, Actuators, and Microsystems*; Anchorage, AK; 21-25 June 2015
- *The 2nd Symposium on Synthesis of Two-dimensional Layered Materials*; Big Sky, MT; 2-7 August 2015
- *2015 Soft Condensed Matter Physics: Self-Assembly and Active Matter GRC/GRS*; New London, NH; 9-14 August 2015
- *Workshop on Non-Linear Spin-Heat Interactions*; Columbus, OH; 16-17 September 2015

5. Special Programs. In FY15, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded five new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Materials Science Division; therefore, all of the Division's active MURIs are described in this section.

1. Materials on the Brink: Unprecedented Transforming Materials. This MURI began in FY07 and was granted to a team led by Professor Kaushik Bhattacharya at the California Institute of Technology. The objective of this research is to develop a fundamental understanding and establish the engineering expertise needed to tailor the electrical, optical, or magnetic (EMO) properties of phase transforming materials through the design and implementation of highly reversible, phase-transformations.

This research is investigating different approaches to achieving highly reversible phase transformations, including such effects as engineered phase compatibility and frustration. The broad selection of material systems (perovskites and multiferroics, Heusler alloys, SMA, and oxy-acid proton conductors), and the design of the studies, will develop a fundamental understanding of the underlying physics that developers need to predict the occurrence of states and the range of behaviors that can be realized within engineered phase transforming materials. The specific goals of this project are to develop and characterize (i) perovskites for electrically tunable photonics and RF-to-optical converters, (ii) metal-ferroelectric multilayers for negative refractive index material applications (a negative surface-plasmon polariton was shown to provide NIM behavior in the visible part of the spectrum), light modulators, thermo-magnetic cooling, spintronics and magnetic field sensing, (iii) shape-memory alloys for large-strain actuators, and (iv) proton-conducting electrolytes for fuel cells. New strategies based on phase engineering of materials have been successfully realized in actuation systems (*e.g.*, in shape memory alloys and relaxor ferroelectrics). These same underlying principles may ultimately be transferable to the development of EM sensors, tunable phase shifters, adaptive optics, optical limiting and energy harvesting devices for use by the Army.

2. Electrical Control of Magnetic Dynamics in Hybrid Metal-Semiconductor Systems. This MURI began in FY08 and was granted to a research team led by Professor Daniel Ralph at Cornell University. The objective of this research is to investigate fundamental phenomena that will enable the all-electrical manipulation of magnetic behavior (both static and dynamic properties) in hybrid structures incorporating magnetic metals, multiferroic oxides and semiconductors.

This research involves fundamental studies on spin injection and transport studies in hybrid metal-semiconductor systems and establish the materials growth and nanofabrication techniques needed to develop a new class of hybrid spin-based electronics. Five studies are being pursued: (i) to study spin injection across metal-semiconductor interfaces, (ii) to develop spin-transfer-torque oscillators and switches, (iii) to pursue the integration of multiferroic materials for electric-field control of exchange coupling bias, (iv) to investigate general approaches to electrical manipulation of spins (electron and nuclear spins), and finally (v) to identify electrical approaches to manipulation of coupled spins in diamond. One key goal is to obtain three orders of increase in the current density of injected spin polarized currents across metal-semiconductor interfaces.

3. Spin-Mediated Coupling in Hybrid Magnetic, Organic, and Oxide Structures and Devices. This MURI began in FY08 and was granted to a team led by Professor Michael Flatte at the University of Iowa. The objective of this research is to investigate fundamental spin-based properties of novel hybrid structures incorporating magnetic metals, multiferroic oxides and organic semiconductors.

This research seeks to develop a new class of hybrid magneto-electronics that can move towards the seamless integration of memory and logic functions under a single device format. The research will conduct some very fundamental studies on spin injection and transport studies in hybrid metal-organic systems. In addition, this work will also look at aspects of nuclear spin imprinting in organics, spin-wave guiding, GHz spin precession and phase locking of sources, OLED modulation, electric-field tuning of spin injection from multiferroic contacts, and electrical switching of ferromagnetism in quasi 2DEG oxide heterostructures. Pioneering studies on magnetoresistance (OMAR) and nuclear spin polarization in organic systems and on conductor-insulator induced transitions in the magnetism of 2DEG oxide heterostructures ($SrTiO_3$ and $LaTiO_3$) are being conducted. It also proposes a very interesting task to use organic overlayers to image the evolution of spin waves from metallic spin torque devices. The program includes a significant theory and modeling task to help guide the experimental effort. As the material capabilities become better defined the program will seek to identify and prototype new device structures relevant to applications in sensors, magnetic storage, dynamic memory and logic, and spin-wave mediated data transfer.

4. Design of Adaptive Load Mitigating Materials Using Nonlinear Stress Wave Tailoring. This MURI began in FY09 and was granted to a team led by Professor John Lambros at the University of Illinois, Urbana. This research is focused on understanding and exploiting wave tailoring phenomena in highly nonlinear inhomogeneous granular media.

The effort builds on recent results demonstrating remarkable dynamic properties in such media, including tunability, energy trapping and wave redirection, primarily because of the highly nonlinear forces that are generated during contact of the granular crystals. Specific granular microstructures will be designed to fully exploit the nonlinear contact effect. Additionally, novel phase transforming ceramics will be fabricated that enhance the granular materials properties by, for example, preferentially strengthening or weakening the material to control local energy dissipation. The specific goals of this research are to (i) incorporate a granular medium in the material system in order to introduce nonlinearity in the material microstructure through local contact between material "elements", thereby furnishing an adaptive and nonlinear targeted energy transfer (TET) capability, (ii) provide additional adaptively coupled with enhanced energy absorption by developing new phase transforming ceramics, (iii) arrange these and other elements in a material system that is either layered (2D), or integrated with a 3D microstructural architecture, and (iv) utilize geopolymers (polymer-like ceramics) to create interfaces that join constituents and also act as "traditional" wave arrestors or reflectors. The comprehensive understanding of propagation and mitigation of high-pressure stress-waves in complex media will guide the future design and demonstration of new materials optimized for high-strain-rate ballistic performance, particularly armor materials. The research is expected to ultimately enable lightweight military hardware with dramatically enhanced survivability, in addition to new paradigms for insensitive munitions.

5. Reconfigurable Matter from Programmable Colloids. This MURI began in FY10 and was granted to a team led by Professor Sharon Glotzer at the University of Michigan - Ann Arbor. This MURI project is co-managed by the Materials Science and the Chemical Sciences Divisions. The goal of this program is to enable the design and synthesis of an entirely new class of self-assembled, reconfigurable colloidal material capable of producing materials with radically increased complexity and functionality. This will revolutionize the ability to build complexity and functionality into materials in the future. Opportunities for manipulating the assembly process include the utilization of shape, intermolecular interactions, induced conformation changes, functionalized adduct and site-specific binding groups, molecule-to-substrate interactions, and external fields. Pathways including both sequential assembly and selective disassembly processes are being investigated. Selective disassembly and reconfigurability are to be accomplished by judicious exposure to heat, pH or light. The research includes aspects of self-limiting growth of superclusters. The experimental program is complemented by a very strong theoretical component. Research thrusts include:

- Sequential staged self-assembly of nano-particles into complex and hierarchical architectures
- Development of theoretical tools and computational algorithms to model the self-assembly process, to identify stable self-assembly pathways that lead to the targeted hierarchical structures, and finally to predict the final properties of the assembled material
- Future derivation of tailored properties and functions within highly complex or hierarchical materials

6. Stress-controlled Catalysis via Engineering Nanostructures. This MURI began in FY11 and was granted to a team led by Professor William Curtin at Brown University. The objective of this research is to prove that macroscopic applied loading can be used to actively control and tune catalytic reactions through the use of innovative nanoscale material systems.

This research is based on the hypothesis that active control using cyclically-applied stress can alleviate the well-established "volcano" effect wherein a desired reaction is optimal only in a narrow operating window due to competing reactions, and thereby overcome what has been believed to be a fundamental limiting factor in design of catalytic systems. The scientific underpinning will be demonstrated by developing two general platforms that can sustain high mechanical loading while also accommodating a range of material systems and catalytic reactions. The main outcome of the project will be the unambiguous proof-of-principle that stress can be used to substantially modify and control chemical reactions, along with possible engineering paths, via both thin film and bulk metallic glass nanostructures for implementing stress control across a wide material space.

7. Atomic Layers of Nitrides, Oxides, and Sulfides (ALNOS). This MURI began in FY11 and was granted to a team led by Professor Pulickel Ajayan at Rice University. The main objective of this MURI is to explore innovative top-down and bottom-up routes for the synthesis or isolation of high quality uni-lamellar sheets and ribbons of nitrides, oxides, and sulfides and to characterization these free standing 2D atomic layers to establish structure-property correlations in 2D layers.

The synthetic approaches of this research will span from simple mechanical/chemical exfoliation techniques to controlled chemical vapor deposition to create various 2D freestanding materials. Researchers will use computational tools based on density functional theory (DFT) methods to investigate binding energies, barriers and stabilities of different dopants and how they affect the band structure of the 2D host materials**.** 2D materials will be characterized for electrical conductivity/resistivity, Hall effect, carrier concentration, mobilities, ionic conductivity and thermal conductivity. If successful, this project could advance the basic science required to develop future DoD applications in chemical and biological sensors, opto-electronics, and power and energy.

8. Translating Biochemical Pathways to Non-Cellular Environment. This MURI began in FY12 and was awarded to a team led by Professor Hao Yan at Arizona State University. This research program is being co-managed by the Life Sciences and Materials Science Divisions. This MURI is exploring how biochemical pathways can potentially function in a non-cellular environment. Cells provide a precisely organized environment to promote maximum efficiency of biochemical reaction pathways, with individual enzymatic components organized via multi-subunit complexes, targeted localization in membranes, or specific interactions with scaffold proteins. The eventual translation of these complex pathways to engineered systems will require the ability to control and organize the individual components outside of the natural cellular environment. Although biological molecules have been successfully attached to inorganic materials, this process often requires chemical modification of the molecule and can restrict its conformational freedom. An alternative approach to maintain biological activity outside of the cell, while preserving conformational freedom, is to encapsulate enzymes within specialized materials or structures. Unfortunately, surface patterning of current encapsulating agents has not achieved the precision required to replicate the organizational capabilities of the cell.

The objective of this research is to develop the scientific foundations needed to design, assemble, and analyze biochemical pathways translated to a non-cellular environment using 3D DNA nanostructures. The MURI team is using DNA nanostructures to direct the assembly of selected biochemical pathways in non-cellular environments. The focus of this research is to develop the scientific foundations needed to translate multienzyme biochemical reaction pathways from the cellular environment to non-biological materials. The ability to translate biochemical reaction pathways to non-cellular environments is critical for the successful implementation of these pathways in DoD-relevant technologies including responsive material systems, solar cells, sensor technologies, and biomanufacturing processes.

9. The Physics of Surface States with Interactions Mediated by Bulk Properties, Defects and Surface Chemistry. This MURI began in FY12 and was awarded to a team led by Prof Robert Cava of the Princeton University. This research is co-managed by the Physics and Materials Science Divisions. The objectives of this project are the discovery, growth, and fabrication of new materials that will display new topologically-stabilized electronic states in both 3D crystals and thin films grown by MBE. Those new materials will be characterized by many different methods including high resolution and spin resolved photoemission spectroscopy, transport, and STM measurements, X-ray scattering, and electron microscopy. The new materials of interest are particularly those that will display interactions arising from the presence of magnetism, such as those based on the heavy metal iridium, and interactions of topological states with superconductivity. State-of the- art materials science methods to optimize the properties of known topological insulators – in particular to enhance the interactions of the surface states with phenomena such as superconductivity are proposed. The correlation of the character of the chemically modified surfaces with the electronic properties will be performed. The team will address new frontiers in physics, such as proximity induced superconductivity in TIs, the 3D TI superconductor CuxBi2Se3, band bending surface capacitance and screening in TIs, and the giant Rashba effect in BiTeI etc.

10. Materials with Extraordinary Spin/Heat Coupling. This MURI began in FY13 and was granted to a team led by Professor Roberto Myers of the Ohio State University. The objectives of this project include understanding the structure-property relationships for coupling heat and spin current in various materials and synthesize magnetic materials with extraordinary and tunable thermal conductivity due to spins, understanding non-equilibrium phonon-magnon transport and the mechanisms behind Spin Seebeck Effect, and finally measuring and understanding phonon-magnon drag and phonon-electron drag in materials.

If successful, this project may lead to long-term applications such as temperature sensors, thermal spintronic devices, solid-state Spin Seebect Effect -based power generators, thermal management in electronic and vehicular applications, and tunable thermal conductivity in materials via magnetic field, microwaves, and light.

11. Theory and Experiment of Cocrystals: Principles, Synthesis and Properties. This MURI began in FY13 and was awarded to a team led by Professor Adam Matzger of the University of Michigan at Ann Arbor. This MURI team is investigating molecular co-crystal formation and the implications for controlling solid-state behavior. This research is co-managed by the Chemical Sciences and Materials Science Divisions.

The largely untapped potential for creating new molecular crystals with optimal properties is just beginning to be realized in the form of molecular co-crystallization. Co-crystallization has the potential to impact the macro-scale performance of many materials, ranging from energetic materials, to pharmaceuticals, to non-linear optics. Unfortunately, the dynamics of molecular co-crystal formation is poorly understood. Molecular co-crystals contain two or more neutral molecular components that rely on non-covalent interactions to form a regular arrangement in the solid state. Co-crystals are a unique form of matter, and are not simply the result of mixing two solid phases. Organic binary co-crystals are the simplest type and often display dramatically different physical properties when compared with the pure ‘parent’ crystals. A significant amount of research on co-crystal design has been carried out by the pharmaceutical industry for the synthesis of pharmaceutical ingredients. However, co-crystal design has not been exploited in broader chemistry and materials science research areas. A recent breakthrough discovery demonstrates that co-crystallization can be used to generate novel solid forms of energetic materials.

The objective of this MURI is to develop a fundamental understanding of intermolecular interactions in the context of crystal packing, and to use the knowledge gained for the design of new co-crystalline molecular materials with targeted, optimized physical and chemical properties. In the long term, a better understanding and control of molecular co-crystallization has the potential to improve the properties of a variety of materials, including: energetic materials, pharmaceuticals, organic semiconductors, ferroelectrics, and non-linear optical materials.

12. Multiscale Mathematical Modeling and Design Realization of Novel 2D Functional Materials. This MURI began in FY14 and was awarded to a team led by Prof Luskin, Mitchell of the University of Minnesota. This research is co-managed by the Mathematics and Materials Science Divisions. The objective of this project is to develop efficient and reliable multiscale methods to couple atomistic scales to the mesoscopic and the macroscopic continuum for layered heterostructures. Layered heterostructures represent a dynamic new field of research that has emerged from recent advances in producing single atomic layers of semi-metals (graphene), insulators (boron nitride) and semiconductors (transition metal dichalcogenides). Combining the properties of these layers opens almost unlimited possibilities for novel devices with desirable, tailor-made electronic, optical, magnetic, thermal and mechanical properties. The vast range of possible choices requires theoretical and computational guidance of experimental searches; experimental discovery can in turn inform, refine and constrain the theoretical predictions.

The proposed research will develop efficient and reliable strongly-linked multiscale methods for coupling several scales based on a rigorous mathematical basis. Specifically: 1) The rigorous coupling of quantum to molecular mechanics will be achieved by properly taking into account the mathematics of aperiodic layered structures. 2) The coupling of atomistic-to-continuum will be achieved by methods that can reach the length scales necessary to include long-range elastic effects while accurately resolving defect cores. 3) New accelerated hybrid molecular simulation methods, specially tailored for the weakly interacting van der Waals heterostructures, will be developed that can reach the time scales necessary for synthesis and processing by CVD and MBE. 4) The simulations will be linked to macro and electromagnetic modelling to understand the physics and bridge to experimental investigation.

The challenge of modeling layered heterostructures will promote the development of strongly-linked multiscale models capable of handling many other materials systems with varied applications, including composites, meta-atoms (atomically engineered structures), and bio-materials that are of interest to the Army.

13. Advanced 2-Dimensional (2D) Organic Networks. This MURI began in FY15 and was granted to a team led by Prof. William Dichtel at Cornell University. The objective of this research is to create stable, free-standing, single-monomer-thick 2D crystalline organic polymer nanosheets/covalent organic frameworks (COFs) with designed electronic (conductivity, mobility, charge storage), optical (resonances, nonlinearities), and structural properties.

The team will combine mechanistic studies, theory, microscopy, and spectroscopy to gain fundamental insight into the 2D polymerization processes. Specifically the team will address the challenges in 2D COF synthesis and characterization by focusing on the following three major research thrusts: (1) exploration of nucleation, bond exchange, and polymerization of 2D COFs to improve their long-range order and morphological form and isolate 2D COFs as single crystals; (2) investigation of new conjugated linkage chemistries, topologies, and doping strategies to impart extensive electronic delocalization and useful optical and electronic properties; and (3) fabrication of new hybrid device heterostructures based on the interfacing of 2D COFs with newly emerging 2D inorganic materials such as transition metal dichalcogenides.

14. Specifically Triggerable Multi-Scale Responses in Organized Assemblies MURI. This MURI began in FY15 and was awarded to a team led by Prof Sankaran Thayumanavan of the University of Massachusetts – Amherst and is being jointly managed by the Materials Science and the Chemical Sciences Divisions. The goal of this effort is to develop a fundamental understanding of how a molecular level detection event can be amplified and then propagated across a macroscopic material to affect a global property change that spans multiple length and time scales. Fundamental approaches for converting single event triggers into extended material responses based on liquid crystal reorientation, regulated amphiphile assembly, gel-to-sol depolymerization and release reactions, and protein-induced transformations are being investigated. A variety of trigger mechanisms based on pH, temperature, redox, light, and enzymatic release are to be developed. A key aspect of this effort is the real-time monitoring of the dynamic changes associated with the cooperative reorganization processes combined with a strong theoretical component aimed at developing models of the material responses and corresponding phase behavior. The breadth of this effort allows for objectives to be pursued in parallel to achieve a fundamental understanding of multi-scale signal propagation and amplification in hierarchical systems and the development of rational design principles for fabricating dynamically responsive material systems.

C. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY15.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY15, the Division managed four new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of two Phase I contracts and two Phase II contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY15 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational

Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY15, the Division managed six new REP awards in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The PECASE winners for each year are typically announced by the White House at the end of the calendar year. However, the FY13-FY15 PECASE recipients had not yet been announced by the end of FY15. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY15, the Division managed four new DURIP projects, totaling $0.8 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. DARPA Nanostructured Materials for Power (NMP) Program

The DARPA NMP program seeks to exploit advanced nano-structured materials for revolutionary improvements in power applications of DoD interest. The ability to decouple and independently control physical, chemical, electromagnetic, and thermal phenomena through nanoscale design, is being tapped to enable improvements in the energy product of permanent magnets and the efficiency of future thermoelectric devices. The Materials Science Division currently co-manages projects within this program. The goals of these projects are ultimately to provide new nano-structured magnetic and thermoelectric materials with enhanced figures of merit for development of higher performance compact power sources in the future.

I. DARPA LoCo Program

The goal of the Local Control of Materials Synthesis (LoCo) program is to develop a low-temperature process for the deposition of thin films whose current minimum processing temperature exceeds the maximum temperature substrates of interest can withstand (e.g., chemical vapor deposited diamond on polymers). The Division currently co-manages projects within this program seeking to realize chemical and physical processes to meet the energetic/chemical requirements of thin film deposition (e.g., reactant flux, surface mobility, reaction energy, etc.), without reliance on broadband temperature input used in state-of-the-art chemical vapor deposition.

J. DARPA Low-Cost Light Weight Portable Photovoltaics (PoP) Program

The goal of the DARPA PoP program is to provide low-cost light-weight portable photovoltaics to DoD. The Materials Science Division currently co-manages projects within this program with the goal of exploring new materials solutions that can meet these goals.

K. DARPA Manufacturing Experimentation and Outreach (MENTOR2) Program

The DARPA MENTOR2 Program seeks to enhance defense readiness by improving both the training and the tools available to those who will be called on to utilize, maintain, and adapt high-technology systems in low-technology environments. MENTOR2 will pursue this goal by developing and demonstrating new training tools, new materials, and new manufacturing technologies in the fields of electromechanical design and manufacturing. It is envisioned that project based curricula employing MENTOR2 design and prototyping tools will teach a deeper understanding of high-technology systems and better enable future competence in the maintenance and adaptation of such systems through the manufacture of as-designed components or the design and manufacture of new components. The Division currently co-manages projects within this program seeking to explore the integration of materials manufacturing and learning approaches to develop and demonstrate new approaches to electromechanical design.

L. DARPA Fracture Putty Program

The DARPA Fracture Putty program seeks to create a dynamic putty-like material which, when packed in/around a compound bone fracture, provides full load-bearing capabilities within days, creates an osteoconductive bone-like internal structure, and degrades over time to harmless by-products that can be reabsorbed as the normal bone regenerates. This new material could rapidly restore a patient to ambulatory function while normal healing ensues, with dramatically reduced rehabilitation time and elimination of infection and secondary fractures. The Division currently co-manages projects within this program attempting to achieve a convergence of materials science, mechanics, and orthopedics to enable new paradigms in bone stabilization, growth, and regeneration.

M. DARPA Structural Logic Program

The DARPA Structural Logic program seeks to enable structural systems that make up the basis for modern military platforms and buildings to adapt to varying loads and simultaneously exhibit both high stiffness and high damping. By demonstrating the ability to combine stiffness, damping, and adaptive dynamic range in a single structure, the Structural Logic program will enable the design of military platforms with the ability to continually change their properties to match the demands of a broad range of dynamic environments. The Division currently co-manages projects within this program seeking to realize novel design paradigms for passively adaptive structural systems that combine high stiffness, damping, and unprecedented adaptability.

N. DARPA Maximum Mobility and Manipulation Program

The DARPA Maximum Mobility and Manipulation program seeks to create and demonstrate significant scientific and engineering advances in robotics that will create a significantly improved scientific framework for the rapid design and fabrication of robot systems and greatly enhance robot mobility and manipulation in natural environments. Additionally, the program seeks to significantly improve robot capabilities through fundamentally new approaches to the engineering of better design tools, fabrication methods, and control algorithms. The Maximum Mobility and Manipulation program covers scientific advancement across four tracks: design tools, fabrication methodologies, control methods, and technology demonstration prototypes. The Division currently co-manages projects within this program seeking to realize novel material design and fabrication paradigms for advanced sensing and actuation materials.

O. DARPA Microphysiological Systems Program

The DARPA Microphysiological Systems program seeks to develop a platform that uses engineered human tissue to mimic human physiological systems. The interactions that candidate drugs and vaccines have with these mimics will accurately predict the safety and effectiveness that the countermeasures would have if administered to humans. As a result, only safe and effective countermeasures will be fully developed for potential use in clinical trials while ineffective or toxic ones will be rejected early in the development process. The resulting platform should increase the quality and potentially the number of novel therapies that move through the pipeline and into clinical care. The Division currently co-manages projects within this program seeking to realize safe and effective countermeasures based upon novel characterization tools, molecular structures, and materials architectures.

P. High Energy Laser Research & Development for HEL-JTO

The High Energy Laser Research & Development Program seeks to support farsighted, high payoff scientific studies leading to advances in HEL science and technology science with the end goal of making HELs lightweight, affordable, supportable, and effective on the modern battlefield. The Division currently manages solid-state laser research of processes and technologies that provide enhancement to the manufacturability of current and innovative design of ceramic gain material.

Q. DARPA Materials for Transduction (MATRIX), DSO-DARPA

Transducer materials convert energy from one form to another, such as thermal to electrical energy, or electric field to magnetic field. While significant progress has been made in advancing energy transducing material performance (e.g. thermoelectrics, multiferroics and phase changing materials) for certain applications, gains at the material level have not always translated into new devices and DoD capabilities. The goal of the MATRIX program is to extend materials breakthroughs to the device and systems level by integrating diverse modeling, design and fabrication communities in a unified research and development effort that bridges the material and the device domains. A major program thrust is the development of multiscale, multimodal design and engineering tools that have the potential to accelerate adoption of MATRIX technology into DoD platforms. The Division currently manages five programs within this DARPA Program:

- Solid State (Gyrator) Device for Low Power Electronics; Dwight Viehland, Virginia Tech.
- Phase-Change Materials Enabling Hyperspectral Imaging: Jeong Moon, HRL
- Wireless Cooling with Caloric Materials: Amy Duwel, Draper Labs
- Tunable Energy Efficient Multiferroic-based Electronics: Shashank Priya, Virginia Tech
- Integrated Magnetoelectric Devices: Carmine Vittoria, Northeastern University

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Materials Science Division.

A. Epitaxial Semiconducting Heusler Alloy Heterostructures

Professor Chris Palmstrøm, University of California - Santa Barbara, Single Investigator Award

The objective of this research is to investigate the hetero-epitaxial growth of semiconducting half-Heusler compounds and study their electronic properties with emphasis on controlling structure and defects. In FY15, the PI successfully grew high crystal quality $Co_{1-x}Ni_xTiSb$ for compositions from x=0 to x=1 and unstrained PtLuSb. Epitaxial $Co_{1-x}Ni_xTiSb$ heterostructures were grown on InGaAs/InP(001), InAlAs/InP(001) and PtLuSb was grown on InAlSb/GaAs(001). He measured the electronic band structure of PtLuSb by ARPES and spin-ARPES where measurements suggest Fermi level lies in the valence band and the presence of a helical spin polarized surface state with linear dispersion crossing the Fermi level, which is suggestive of a topological surface state (see FIGURE 1). Metal-to-insulator transition of $Co_{1-x}Ni_xTiSb$ was investigated using ARPES and temperature dependent electrical transport. The carrier concentration was reduced from ~10^{20} to mid-10^{17} carriers/cm^3 in CoTiSb by controlling the point defects allowing for mobilities in excess of 500 cm^2/Vs at room temperature, which are comparable to Si for similar carrier densities.

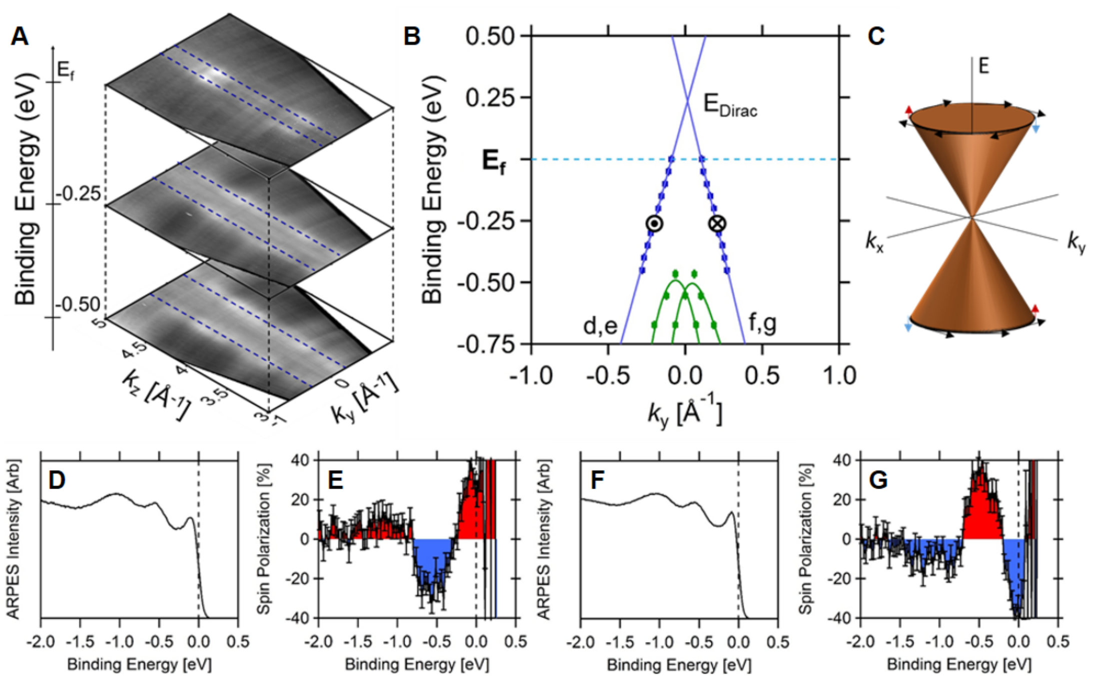

FIGURE 1

Band structures suggestive of topological surface state. (**A**) Out-of-plane momentum dependence for various binding energies. An absence of kz dispersion is observed, consistent with the behavior of a surface state. (**B**) By tracking this state's position as a function of binding energy, a Dirac-like behavior can be seen with a crossing point approximately 235 meV above the Fermi level. Spin-ARPES spin polarization directions are marked. (**C**) Schematic diagram of a topological surface state with helical spin texture. (**D-E**,**F-G**) ARPES intensity and corresponding spin polarization for the left and right side of the linearly dispersing surface state, respectively. A counter-clockwise helical spin texture, consistent with a topological surface state, is observed.

B. Novel Phenomena in Ferroelectrics

Professor Laurent Bellaiche, University of Arkansas, Single Investigator Award

The goal of this research is to investigate various static and dynamical properties of low-dimensional ferroelectrics and multiferroics (and related materials) to discover novel phenomena of large fundamental and technological importance in these nanostructures. To reach this goal, the PI developed and used first-principles-based schemes, and collaborated extensively with International experimental scientists. In FY15, the PI achieved the first discovery of stable electrical skyrmionic state in ferroelectric nanocomposites (see FIGURE 2). In this work, the PI demonstrated, via the use of a first-principles-based framework, that skyrmionic configuration of polarization can be extrinsically stabilized in ferroelectric nanocomposites. The interplay between the considered confined geometry and the dipolar interaction underlying the ferroelectric phase instability induces skyrmionic configurations. The topological structure of the obtained electrical skyrmion can be mapped onto the topology of domain-wall junctions. Furthermore, the stabilized electrical skyrmion can be as small as a few nanometers, thus revealing prospective skyrmion-based applications of ferroelectric nanocomposites.

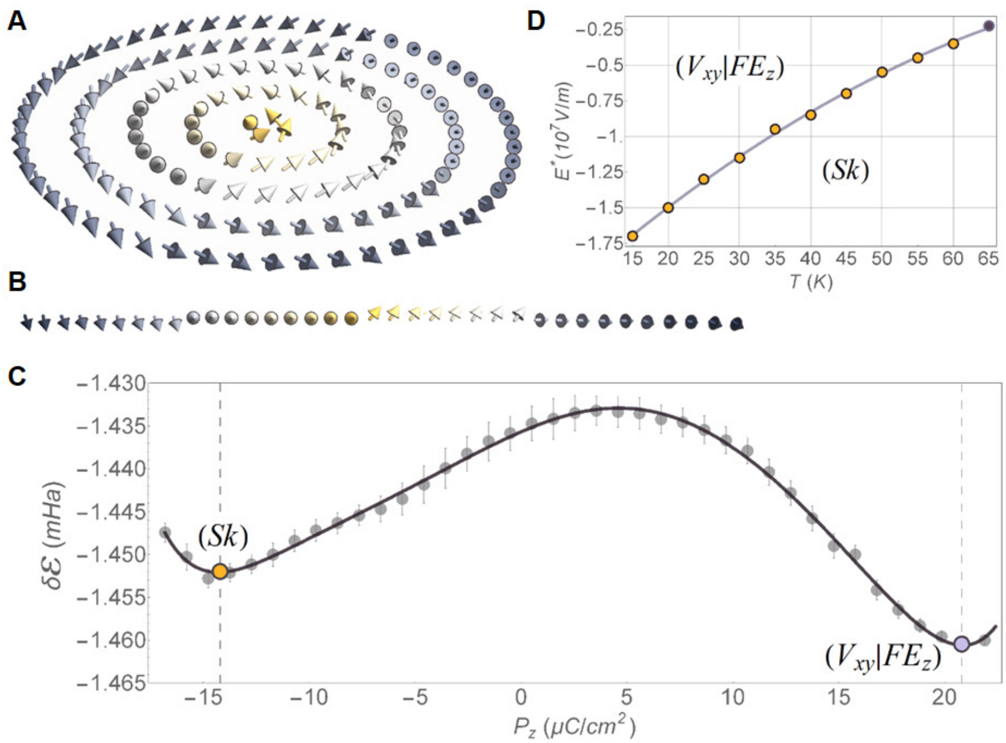

FIGURE 2

Stability of the skyrmionic state. (A) Polarization field configuration within the relaxed skyrmionic state (Sk) as obtained from the simulation at 15 K. (B) Local dipoles plotted along a line passing through the skyrmion's core and parallel to the x coordinate axis. It is seen that the tips of the dipoles describe a circle in the plane perpendicular to the line, thus indicating the variation of the y and z components along this line. The vectors are coloured according to their z-component in A,B. (C) Dependence of the internal energy de on the Pz component of polarization showing the crossover between two stable minima: the one corresponding to the (Vxy|FEz) state characterized by a vortex pattern in the z-planes co-occurring with an electrical polarization along the [001] direction, and the one associated with the skyrmionic texture (Sk). Error bars indicate s.d. (D) Temperature dependence of the estimated threshold external electric field E* needed to drive the system towards the skyrmion state.

This discovery may surpass all commercially-available magnets except for the neodymium magnets that are of little utility to the DoD because of their relatively low maximum operating temperature. This breakthrough represents the first critical step in the development of a new generation of rare-earth element-free hard magnetic materials. An added advantage of this class of magnet is that they will have good high thermal stability and oxidation resistance which should permit operation at temperatures far above those of current magnets.

C. Reconfigurable DNA Assembly Processing
Professor David Pine, New York University, MURI Award

DNA-coated colloids hold great promise for self-assembly of programmed heterogeneous microstructures, provided they not only bind when cooled below their melting temperature, but also rearrange so that aggregated particles can anneal into their most stable (minimum energy) structures. Unfortunately, when the thickness of the DNA coating is much smaller than the particles, the DNA-coated particles generally collide and stick forming kinetically arrested random aggregates. Interestingly, in FY15, the research team reported on DNA-coated colloids that can rearrange and anneal, and thus, for the first time, enable the growth of dense colloidal assemblies with particulate densities approaching 85% (versus typical values of ~ 5%). The process involves coating µm-sized particles uniformly with short DNA linker molecules and then growing and annealing aggregate materials from a bath of complementary DNA-coated particles held at temperatures just below the melting point of the starting colloids (see FIGURE 3). The process enables the growth of dense colloidal crystals with engineered crystal structures and symmetries that go beyond traditional close-packed geometries. The kinetics of aggregation, crystallization and defect reduction were tracked in real time and found to be possible only within a very narrow window of temperature just below the melting point of the colloids.

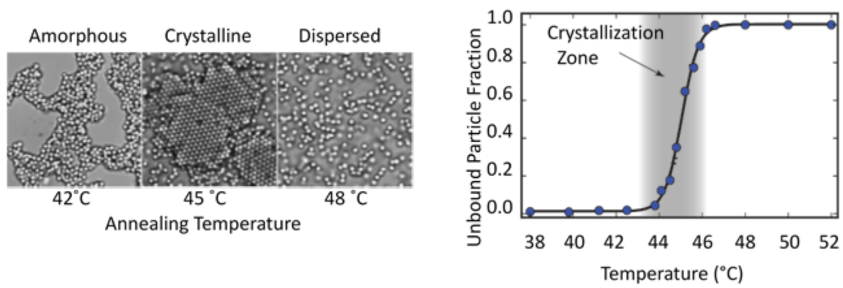

FIGURE 3

Crystallization of DNA-coated particles. Bright-field optical images showing the morphologies of DNA-coated 1.0-micron diameter particle assemblies as a function of annealing temperature, showing a narrow window where particle crystallization occurs.

D. Majorana Fermions Observed
Professor Ali Yazdani, Princeton University, Single Investigator Award

Majorana fermions have been predicted to localize at the edge of a topological superconductor, or a state of matter that can form when a ferromagnetic system is placed in proximity to a conventional superconductor with strong spin-orbit interactions. In FY15, scanning tunneling conductance measurements on just such a system were recently performed by researchers at Princeton headed by Professor Ali Yazdai. To realize a one-dimensional topological superconductor, the group placed atomic chains of ferromagnetic iron (Fe) on the surface of superconducting lead (Pb). Using high-resolution spectroscopic imaging techniques, they showed that the onset of superconductivity, which gaps the electronic density of states in the bulk of the Fe chains, is accompanied by the appearance of zero-energy end-states (see FIGURE 4). This spatially resolved signature provided the first strong evidence, corroborated by other observations, for the formation of a topological phase and edge-bound Majorana fermions within the atomic chains.

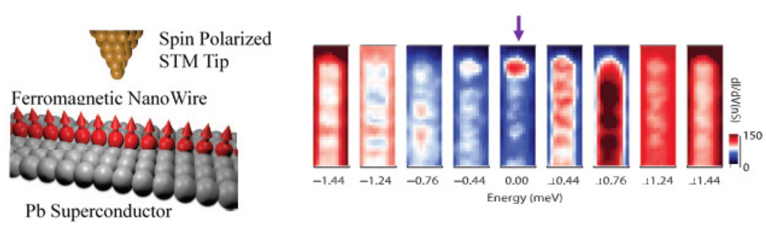

FIGURE 4

Schematic of experimental setup (left) and spectroscopic mapping of atomic chains and observation of zero-energy end states (arrow) indicative of Majorana Fermions.

E. Nanoparticles Create Uniform Dispersion of Bismuth in Immiscible Alloys
Professor Xiaochun Li, University of California - Los Angeles, Single Investigator Award

The goal of this research is to develop a method to control the growth and distribution of a minority phase in a bulk immiscible alloy. Immiscible alloys contain elements that do not alloy upon cooling from high temperature, instead separating into two phases. In the Zn-Bi system, the density difference between the elements and the rapid growth of Bi droplets cause the Bi phase to separate to the bottom of castings, resulting in an inhomogeneous distribution (see FIGURE 5A). In FY15, researchers at the University of California - Los Angeles utilized nanoparticles to control the size and dispersion of the Bi phase in both the Al-Bi and Zn-Bi systems. When the nanoparticles ($TiC_{0.7}N_{0.3}$ for Al and W for Zn) were introduced by the researchers into the immiscible alloy melt, they coated the surface of the Bi droplets that formed upon cooling. This coating created an interface that impaired diffusional transport and limited droplet coagulation. As a result, the Bi droplets are finer in size, reducing their tendency to settle to the bottom of the alloy. The researchers found that when the nanoparticles are used the Bi is more uniformly distributed in the alloy (see FIGURE 5B). These nanoparticle controlled immiscible alloys constitute an opportunity for superior bearing materials due to their ability to self-lubricate. The nanoparticle method could also be adapted for use in other material systems to create immiscible bulk alloys with unique physical or electromagnetic properties.

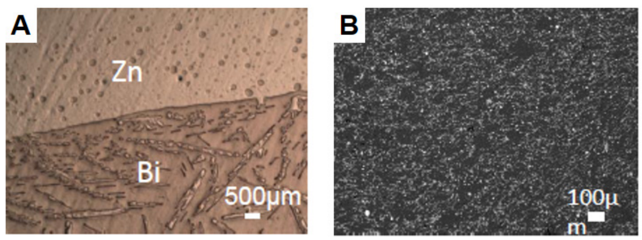

FIGURE 5

Zn-Bi alloy with or without W nanoparticles. (**A**) Zn-Bi alloy without W nanoparticles, where the Zn and Bi phases have separated into two separate regions. (**B**) Zn-Bi alloy with W nanoparticles added, where the Bi-phase is more uniformly distributed in the Zn matrix.

F. Microstructural Model of Ag/Cu Interfaces Subjected to Compressive Stress
Professor Izabela Szlufarska, University of Wisconsin-Madison, Single Investigator Award

The objective of this research is to develop a numerical method that accurately simulates the response of metals subjected to sliding contact. The complexity of the underlying mechanics requires the simultaneous use of molecular dynamics, phase field, and finite element modeling to accurately simulate the relevant mechanical forces and microstructural evolution of the metal. In FY15, researchers at the University of Wisconsin-Madison integrated these different modeling methods into a single simulation via the MOOSE/MARMOT software platform in order to accurately simulate grain boundary plasticity. This was accomplished by implementing a stress interpolation scheme into the phase field model that properly calculated the stresses at the grain boundaries. The adjusted phase field model simulated the motion of the grain boundaries during a sliding contact and the resulting effect this had on dislocation density and activity. The model was used to study the response of the two types of interface in a Cu/Ag alloy, twin and cube-on-cube, to a compressive stress. Molecular dynamic simulations were used to simulate the interfaces and were validated by TEM observations. It was found that the twin interfaces impaired dislocation motion, resulting in a dislocation pile up at the interface when the compressive stress was applied. The improved understanding of the underlying mechanics of sliding contact provided by this simulation will enable the development of materials with superior wear resistance.

G. Guiding Stress Waves through Stress-Induced Domain Switching
Professors Julian Rimoli and Massimo Ruzzene, Georgia Institute of Technology, Single Investigator Award

The objective of this research is to explore and demonstrate the management of stress waves with periodic, graded and domain switching multiphase materials. The research has focused recently on the analysis of stress wave propagation in undulated beams and plates, as a means of providing a robust set of fabricated metamaterials with wave-steering properties. In undulated beams, curvature couples longitudinal and bending behavior, resulting in complete band gaps open for nonzero curvature, where wave propagation is forbidden. Furthermore, band gap width increases with both undulation and beam thickness. In undulated plates, local curvatures couple in-plane and out-of-plane behavior, resulting in modal band gaps where only shear waves are allowed, while flexural and compressive waves are forbidden. The width of the modal band gap increased with undulation but decreased with plate thickness. In FY15, the team designed metamaterials based on undulated lattices (*i.e.*, band gaps in these kind of metamaterials can be modulated through lattice waviness and thickness), with results demonstrating that spatial grading in undulation parameters led to non-uniform metamaterial directionality that can be exploited to gradually steer stress waves (see FIGURE 6).

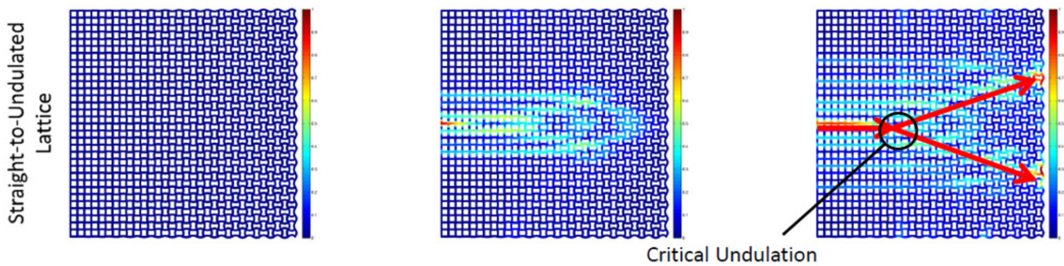

FIGURE 6

Spatial grading in undulation parameters leads to non-uniform metamaterial directionality, which can be exploited to gradually steer stress waves.

H. First Thin-Film-Processable High Ionic Conductivity Cationic Polymers

Professor Andrew Herring, Colorado School of Mines, MURI Award

The objectives of this research are to produce revolutionary, robust, durable, thin anion exchange membranes with sufficiently high ionic conductivities for practical devices, and to fundamentally understand, with combined experimental and computational approaches, the interplay of chemistry, processing, and morphology on the performance and durability of anion exchange membranes. In FY15, the researchers developed unique co-polymers based on ethylene and isoprene with cationic units for mechanically stable AEMs, and successfully processed these materials into large area thin films approximately 10 micrometers in thickness (see FIGURE 7). This result was achieved through the simultaneous and integrated design of novel polymers, polymer architectures and optimized structure-property relationships. In particular, the work has focused on co-polymers of vinylbenzyltrimethylammonium, PVBTMA, as these are readily synthesized as organized or random di-block polymers. This choice enables a wide range of architectures, direct characterization of functionality and in-silico simulation so that predictive modeling can be used to optimize next generation materials.

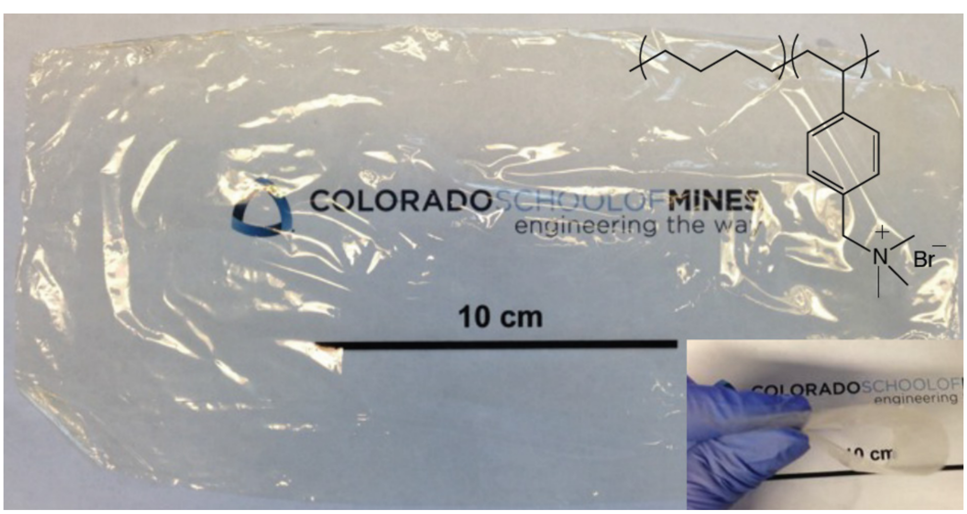

FIGURE 7

Example of ~300 cm^2 flexible PE-b-PVBTMA[Br] film after casting and functionalization, with a consistent thickness of 10-15 µm.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Hexagonal Atomic Sheets of Silicon (Silicene)

Investigator: Professor Deji Akinwande, University of Texas - Austin, Single Investigator Award
Recipients: ARL-SEDD, U.S. Army Armament Research, Development and Engineering Center (ARDEC)

The objective of this research is to grow 2-dimensional (2D) free-standing silicon (silicene) through basic understanding of nucleation and the growth and explore fundamental device properties such as charge transport, charge injection across interfaces and contact resistance etc. The PI discovered that Ag/Mica substrate stack facilitates the epitaxial growth of silicene and developed an innovative process to transfer silicene after growth on to insulating substrates for further encapsulation and device fabrication (see FIGURE 8). He was able to demonstrate for the first time electric field-effect control of silicene proving its predicted Dirac properties. This project was done in collaboration with ARL-SEDD, and the results transitioned to ARDEC and ARL-SEDD to identifying properties of these novel 2D materials for future Army technologies.

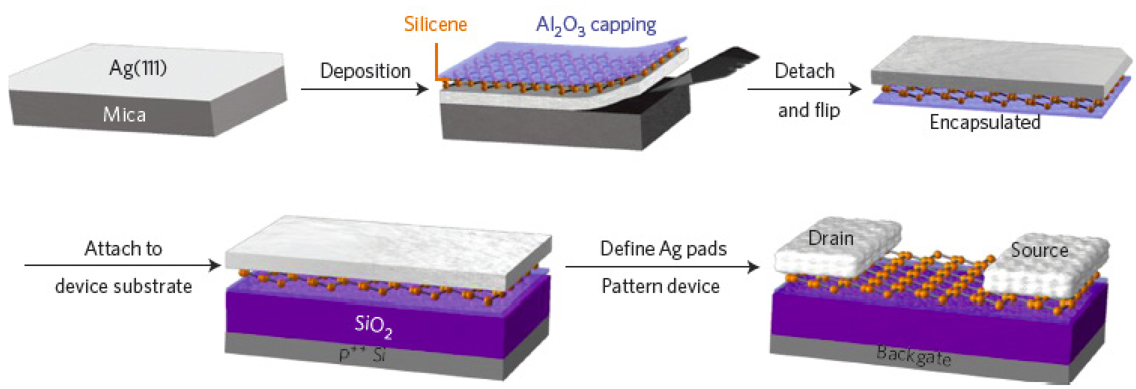

FIGURE 8

Silicene Encapsulated Delamination with Native Electrode (SEDNE). The invention of the new transfer method SEDNE includes the following key steps: epitaxial growth of silicene on crystallized Ag(111) thin film on mica, in-situ Al_2O_3 capping, encapsulated delamination transfer of silicene, and native contact electrodes formation to enable back-gated silicene transistors for the first time.

B. Super-Resolution Optical Imaging

Investigator: Professor Vasily Astratov, University of North Carolina - Charlotte, Single Investigator Award
Recipient: Air Force Research Laboratory

Microsphere-assisted optical imaging techniques developed by researchers at the University of North Carolina - Charlotte transitioned to the Sensors Division at the Air Force Research Laboratory in FY15. The technology has demonstrated several advantages over related confocal and solid immersion lens microscopies, including intrinsic flexibility, better resolutions, higher magnifications, and longer working distances. To date, the researchers have been able to resolve minimal feature sizes in nano-plasmonic arrays down to about 50-60 nm (or $\lambda/7$) by imaging through 15μm diameter barium titanate glass spheres (n~1. 9) immersed in isopropyl alcohol (n~1. 37) using illumination wavelengths of λ=405 nm. By extending the approach to deep UV wavelengths (~200 nm) they estimate that they should be able to image nanostructures with extraordinary high resolutions approaching ~30 nm.

C. Fabrication of High Performance Mg/MAX phase Composites
Investigator: Professor Michel Barsoum, Drexel University, Single Investigator Award
Recipient: ARDEC

Previous research at Drexel led to the discovery of the MAX family of materials. MAX materials are machinable and layered ternary carbides or nitrides. MAX is an abbreviation of general formula $M_{n+1}AX_n$, where M is an early transition metal, A is an A-group element, and X is either C and/or N. When the MAX composition Ti_2AlC was introduced into Mg, a nanostructured Mg-MAX composite with remarkable mechanical properties was formed. Further development of these composites was supported by ARO, cumulating in the development of a MAX/Mg composite with a compressive strength of >1GPa. In FY15, a cooperative research and development agreement (CRADA) was established between Drexel and ARDEC. Under the terms of the CRADA, ARDEC will provide specifications for the materials, identify programs that can benefit from the technology, and help Drexel scale-up the process. Drexel will continue to develop the composites in order to meet ARDEC's needs and will perform the research necessary to enable the eventual commercial production of these materials. This technology could lead to the development of new lightweight materials for armor, weapons, and energetic applications.

D. Toughened 3D Printed Polymeric Structures
Investigator: Professor Micah Green, Texas A&M University, STIR Award
Recipients: National Aeronautics and Space Administration (NASA)

The objective of this short-term research effort is to investigate the microwave-induced heating response of polymer composites containing carbon nanotube (CNT) fillers. More specifically, the aim is to characterize the thermal response of percolated multi-walled carbon nanotube (MWCNT)/polymer composites to microwave irradiation, and to demonstrate microwave-induced polymer adhesion due to nanoscale localized welding. In FY15, joint research efforts were initiated with NASA to provide advanced tensile testing and controlled microwave exposure of 3D printed CNT-welded polymeric materials to enhance this effort. The collaboration identified that non-uniform microwave exposure caused localized "cold spots" which disrupted the tensile improvement, a critical design consideration for future optimized 3D printed materials.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Spin Polarized Transparent Conductors through Complex Oxide Epitaxy

Professor Yuri Suzuki, Stanford University, Single Investigator Award

The objective of this research is to develop a new class of spin polarized transparent conductors through cation doping in epitaxial stannate oxide thin films (e.g., Gd doped BaSnO3) . The PI will address materials challenges associated with combining transparency, metallicity and magnetism as well as the origin of ferromagnetism in these transparent oxides. It is anticipated that in FY16, the research team will design and synthesize stannate-based spin polarized transparent conductors with ordered cation defects. In future years, the team will complete local structural, electronic and magnetic characterization via x-ray absorption spectroscopy, x-ray magnetic circular dichroism, photoemission electron microscopy, x-ray resonant magnetic scattering, magnetic force microscopy, transmission electron microscopy and electron energy loss spectroscopy.

B. Dynamic Nuclear Polarization Realized for Magnetic Resonance Force Microscopy

Professor John Marohn, Cornell University, Single Investigator Award

The objective of this research at Cornell University is to continue to improve on the performance of their magnetic resonance force microscope. It is expected that in FY16, the research team will demonstrate dynamic nuclear polarization techniques that will significantly improve on the sensitivity of their current system. This will open the way for high-resolution 3D magnetic resonance imaging of biological systems, which will afford a new look at cellular chemistry and processes. The ultimate goal of the program is to reach sensitivities that will provide for magnetic resonance imaging of single nuclear spins.

C. Creation of a Copper-Carbon Nanotube Composite Aerogel

Professor Mohammad Islam, Carnegie Mellon University, Single Investigator Award

The objective of this research effort is to fabricate nano-grained copper composites with a uniform dispersion of a reinforcing carbon nanotube (CNT) network. The researchers recently applied Cu coatings to CNT aerogels via solution based impregnation, demonstrating that a Cu coating could be adhered to a CNT network. In FY16, it is anticipated that a unique Cu/CNT composite with a uniform dispersion of CNTs will be fabricated, establishing a novel process for stabilizing nano-sized grains in metals that could be applied to other composite systems.

D. Dynamics of a Monolayer of Microspheres on an Elastic Substrate

Professor Nicholas Boechler, University of Washington, YIP Award

The objective of this research effort is to utilize a combined theoretical, computational, and experimental approach to study high strain rate shock wave propagation and the resulting failure self-assembled three-dimensional granular media. This combined approach uniquely simplifies the problem via ordered granular media, while maintaining relevance via micro- to nanoscale grains, in order to dramatically enhance the understanding of the dynamics of granular media and transform the way granular media is studied. In FY16, the research will seek to capture the dynamics of a discrete monolayer of spheres adhered to an elastic substrate through a combination of discrete and effective medium models that could predict scalable results for use with nano- to macroscale systems.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. David Stepp
Division Chief
Program Manager, Mechanical Behavior of Materials
Program Manager (Acting), Synthesis and Processing of Materials

Dr. John Prater
Program Manager, Materials Design

Dr. Chakrapani (Pani) Varanasi
Program Manager, Physical Properties of Materials

Dr. Julia Barzyk
Program Manager, Earth Materials and Processes

B. Directorate Scientists

Dr. David M. Stepp
Director (Acting), Engineering Sciences Directorate

Dr. April Brown (IPA)
Research Scientist

Mr. George Stavrakakis
Contract Support

C. Administrative Staff

Ms. Pamela Robinson
Administrative Support Assistant

CHAPTER 8: MATHEMATICAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2015* is to provide information on the programs and basic research supported by ARO in fiscal year 2015 (FY15), and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Mathematical Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY15.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Mathematical Sciences Division supports research to develop a foundational framework for the understanding and modeling of complex nonlinear systems, for stochastic networks and systems, for mechanistic models of adaptive biological systems and networks, and for a variety of partial differential equation (PDE) based phenomena in various media. These research areas focus on discovering nonlinear structures and metrics for modeling and studying complex systems, creating theory for the control of stochastic systems, spatial-temporal statistical inference, data classification and regression analysis, predicting and controlling biology through new hierarchical and adaptive models, enabling new capabilities through new bio-inspired techniques, creating new high-fidelity computational principles for sharp-interface flows, coefficient inverse problems, reduced-order methods, and computational linguistic models. This research will ensure the U.S. is on the research frontier in mathematical sciences, and will enable new advances in disciplines that depend on mathematics.

2. Potential Applications. Research managed by the Mathematical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. Long term basic research discoveries regarding the modeling of complex systems may enable full (*i.e.*, not only physical) situational awareness through modeling of urban terrain and small-group social phenomena. Outcomes of basic research in probability and statistics may provide enhanced levels of information assurance, improved awareness of and defense against terrorist threats, next generation communication networks, and improved weapon design, testing, and evaluation. New discoveries in biomathematics may lead to protection against future biological and chemical warfare agents, improve wound-healing, lead to self-healing communication networks, enhance cognitive capabilities for the Soldier, and contain or prevent infectious disease. Advances from basic research in the area of numerical analysis may enable faster/better analysis, design, prediction, real-time decision making, and failure autopsy.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives and to maximize the impact of potential discoveries for the Army and the nation, the Mathematical Sciences Division frequently coordinates, leverages, and transitions research within its Program Areas with Army scientists and engineers, such as the ARL Weapons and Materials Research Directorate (ARL-WMRD) and ARL Sensors and Electron Devices Directorate (ARL-SEDD), and also other DoD agencies such as the Office of Naval Research (ONR) and the Air Force Office of Scientific Research (AFOSR). In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multi-disciplinary research topics, and evaluate the effectiveness of research approaches. For example, interactions with the Network Sciences Division pursue common interests in cognitive modeling, bio-network modeling and design, and new concepts in computational optimization. The Mathematical Sciences Division also coordinates its research portfolio with the Computing Sciences Division to promote investigations of new architectures and algorithms for the future of heterogeneous computing and to pursue related interests in image recognition and information fusion. Research also complements initiatives in the Life Sciences Division to model and understand the relationship between microbial growth conditions and composition, leading to advances in microbial forensics. The creation of new computational methods and models to better understand molecular structures and chemical reactions are an area of collaboration between the Chemical Sciences and Mathematical Sciences Divisions. The Mathematical Sciences Division also coordinates its research portfolio with the Physics Division to pursue fundamental research in quantum control. The Division interfaces with Program Areas in the Mechanical Sciences Division to explore the mechanics of fluids in flight and to better understand combustion. These interactions promote synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

B. Program Areas

The Mathematical Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY15, the Division managed research within these four Program Areas: (i) Modeling of Complex Systems, (ii) Probability and Statistics, (iii) Biomathematics, and (iv) Computational Mathematics. As described in this section and the Division's BAA, these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Modeling of Complex Systems. The goal of this Program Area is to develop quantitative models of complex, human-based or hybrid physics and human-based phenomena of interest to the Army by identifying unknown basic analytical principles and by using human goal-based metrics. Complete and consistent mathematical analytical frameworks for the modeling effort are the preferred context for the research, but research that does not take place in such frameworks is considered if the phenomena are so complex that such frameworks are not feasible. The identification of accurate metrics is part of the mathematical framework and is of great interest, as traditional metrics often do not measure the characteristics in which observers in general, and the Army in particular, are interested. For many complex phenomena, new metrics need to be developed at the same time as new models. This Program Area is divided into two research thrusts: (i) Geometric and Topological Modeling and (ii) Small-group Social and Sociolinguistic Modeling. In FY13, the Modeling of Complex Systems Program included legacy efforts in information fusion. New efforts in information fusion will be part of the Information Processing and Fusion Program in the ARO Computing Sciences Division.

This Program Area develops mathematical analysis for fully 3D (rather than 2.5D) geometric and topological modeling of large urban regions up to 100 km x 100 km, which is important for situational awareness, mission planning and training. It develops the quantitative, analytical models of small social groups and of sociolinguistic phenomena which are required for operations, training, simulation (computer generated forces) and mission planning.

2. Probability and Statistics. The goal of this Program Area is to create innovative theory and techniques in stochastic/statistical analysis and control. Basic research in probability and statistics will provide the scientific foundation for revolutionary capabilities in counter-terrorism, weapon systems development, and network-centric warfare. This Program Area is divided into two Thrust areas: (i) Stochastic Analysis and Control, and (ii) Statistical Analysis and Methods.

The goal of the Stochastic Analysis and Control Thrust is to create the theoretical foundation for modeling, analysis, and control of stochastic networks, stochastic infinite dimensional systems, and open quantum systems. Many Army research and development programs are directed toward modeling, analysis, and control of stochastic dynamical systems. Such problems generate a need for research in classical and quantum stochastic processes, random fields, and/or classical and quantum stochastic differential equations in finite or infinite dimensions. These systems often have non-Markovian behavior with memory for which the existing stochastic analytic and control techniques are not applicable. The research topics in this Thrust include, but are not limited to, the following: (i) analysis and control of stochastic delay and partial differential equations; (ii) complex and multi-scale networks; (iii) spatial-temporal event pattern analysis; (iv) quantum stochastics and quantum control; (v) stochastic pursuit-evasion differential games with multi-players; and (vi) other areas that require stochastic analytical tools.

The objective of the Statistical Analysis and Methods Thrust is to create innovative statistical theory and methods for network data analysis, spatial-temporal statistical inference, system reliability, and classification and regression analysis. The research in this Thrust supports the Army's need for real-time decision making under uncertainty and for the design, testing and evaluation of systems in development. The following research topics are of interest to the Army and are important for providing solutions to Army problems: (i) Analysis of very large or very small data sets, (ii) reliability and survivability, (iii) data, text, and image mining, (iv) statistical learning, (v) data streams, and (vi) Bayesian and non-parametric statistics, (vii) statistics of information geometry, and (viii) multivariate heavy tailed statistics.

Potential long-term applications for research carried out within this Program Area include optimized design and operation of robust and scalable next-generation mobile communication networks for future network-centric operations made possible through advances in stochastic network theory and techniques. Also, advances in stochastic fluid turbulence and stochastic control of aerodynamics can improve the maneuvering of helicopters in adverse conditions and enable optimal design of supersonic projectiles. In addition, new results in density estimation of social interactions/networks will help detect adversarial behaviors and advances in spatial-temporal event pattern recognition and will enable mathematical modeling and analysis of human hidden intention and will provide innovative approaches for counter-terrorism and information assurance. Finally, new discoveries in signature theory will significantly improve reliability of Army/DoD systems and experimental design theory, and will lead to accurate prediction and fast computation for complex weapons.

3. Biomathematics. The goal of this Program Area is to identify and mathematize the fundamental principles of biological structure, function, and development across biological systems and scales. The studies in this program may enable revolutionary advances in Soldier health, performance, and materiel, either directly or through bio-inspired methods. This Program Area is divided into three main research Thrusts: (i) Multiscale Modeling/Inverse Problems, (ii) Fundamental Laws of Biology, and (iii) Modeling Intermediate Timescales. Within these thrusts, basic, high-risk, high pay-off research efforts are identified and supported to achieve the program's long-term goals. Research in the Multiscale Modeling/Inverse Problems Thrust involves creating mechanistic mathematical models of biological systems at different temporal and/or spatial scales and synchronizing their connections from one level of organization to another, with the goal of achieving a deeper understanding of biological systems and eventually connecting top-down and bottom-up approaches. Research in the Fundamental Laws of Biology Thrust is high-risk research in biomathematics at its most fundamental level, seeking to find and formulate in a mathematical way the basic, general principles underlying the field of biology, a feat that has been performed for other fields, such as physics, but is in its infancy with respect to biology. Efforts in the Modeling at Intermediate Timescales Thrust attempt to develop new methods of modeling of biological systems, as well as their control, at intermediate timescales.

While these research efforts focus on high-risk, high pay-off concepts, potential long-term applications for the Army include new and better treatments for biowarfare agent exposure, improved military policies on troop movements in the presence of infectious disease, optimized movements of groups of unmanned autonomous vehicles and communications systems, and improved understanding of cognition, pattern recognition, and artificial intelligence efforts. Research in this Program Area could also lead to improved medical diagnoses, treatments for disease, limb regeneration, microbial forensics, detection of terrorist cells, and self-healing networks. Finally, efforts within this program may result in a revolutionized understanding of biology in general, which will at the very least allow future modeling efforts to be much more efficient and also undoubtedly have far-reaching effects for the Army in ways yet to be imagined.

4. Computational Mathematics. The goal of this Program Area is to develop a new mathematical understanding to ultimately enable faster and higher fidelity computational methods, and new methods that will enable modeling of future problems. The research conducted within this program will enable the algorithmic analysis of current and future classes of problems by identifying previously unknown basic computational principles, structures, and metrics, giving the Army improved capabilities and capabilities not yet imagined in areas such as high fidelity modeling, real-time decision and control, communications, and intelligence. This Program Area is divided into three research Thrusts: (i) Multiscale Methods, (ii) PDE-Based Methods, and (iii) Computational Linguistics. Within these Thrusts, high-risk, high pay-off research efforts are identified and supported to pursue the program's long-term goals. The goal of research in the Multiscale Methods Thrust is to achieve higher fidelity and more efficient modeling of multiscale phenomena in a variety of media, and to create general methods that make multiscale modeling accessible to general users. Efforts in the PDE-Based Methods

Thrust focus on developing the mathematics required for higher fidelity and more efficient modeling of sharp-interface phenomena in a variety of media, to discover new methods for coefficient inverse problems that converge globally, and to create reduced order methods that will achieve sufficiently-accurate yet much more efficient PDE solutions. Efforts in the Computational Linguistics Thrust focus on creating a new understanding of natural language communication and translation through new concepts in structured modeling.

While these research efforts focus on high-risk, high payoff concepts, potential long-term applications for the Army include force protection concrete and improved armor, more stable but efficient designer munitions, high density, rapid electronics at low power, and nondestructive testing of materials. Program efforts could also lead to more capable and robust aerial delivery systems, more efficient rotor designs, systems to locate explosive materials, more efficient combustion designs, and real-time models for decision-making. Finally, efforts within this program may lead to natural language interactions between bots and humans in cooperative teams, new capabilities for on-the-ground translation between deployed U.S. forces and locals, especially in low-resource language regions, new and improved capabilities for automated translation, automatic summarization, and textual analysis within the strategic intelligence communities.

C. Research Investment

The total funds managed by the ARO Mathematical Sciences Division for FY15 were $21.6 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY15 ARO Core (BH57) program funding allotment for this Division was $5.5 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $7.7 million to projects managed by the Division. The Division also managed $0.9 million of Defense Advanced Research Projects Agency (DARPA) programs, $1.8 million of Congressional funds, and $0.8 million was provided by other Army Laboratories. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $1.9 million for contracts. Finally, $3.0 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.3 million of ARO Core (BH57) funds, in addition to any funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY15 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY15 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY15, the Division awarded 21 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Animashree Anandkumar, University of California - Irvine; *Development of Large-Scale Tensor Libraries for Machine Learning*
- Professor Luke Bornn, Harvard University; *Statistical Structural Health Monitoring in the Presence of Environmental Variability and Uncertainty*
- Professor Robert Elliott, The University of Adelaide; *Filtering Using Non-linear Expectations*
- Professor Timothy Elston, University of North Carolina - Chapel Hill; *Spatio-temporal Control of Rho Family Signaling Networks in Motility*
- Professor Shu-Cherng Fang, North Carolina State University; *L1 – Based Major Component Detection and Analysis for n-Dimensional Data Clouds Based on Linear Conic Programming*
- Professor John Foster, University of Texas at Austin; *Nonlocal and Fractional Order Methods for Near-wall Turbulence, Large-eddy Simulation, and Fluid-structure Interaction*
- Professor Vikram Gavini, University of Michigan - Ann Arbor; *Numerical Methods and Scalable Algorithms for Large-scale Real-space Time Dependent Density Functional Theory Calculations*
- Professor Jean-Luc Guermond, Texas A&M University; *Finite Element Approximation of Nonlinear Systems Developing Shocks, Fronts and Interfaces*
- Professor Udita Katugampola, University of Delaware; *Can Fractional Order Models do more Justice to Anomalous Behavior than Familiar Classical Order Models?*
- Professor Michael Klibanov, University of North Carolina - Charlotte; *Globally Convergent Inverse Algorithms via Carleman Weight Functions: Theory, Numerical Studies and Experimental Verifications*
- Professor Eric Kolaczyk, Boston University; *Statistical Foundations for Analyzing Large Collections of Network-data Objects*
- Professor Gangaram Ladde, University of South Florida; *Network-Centric Stochastic Hybrid Dynamic Time-Event Process Modeling, Methods, and Analysis*

- Professor Daniel Lidar, University of Southern California; *Control of Quantum Open Systems: Theory and Experiment*
- Professor Jingchen Liu, Columbia University; *Rare-event Analysis and Computational Methods for Stochastic Systems Driven by Random Fields*
- Professor Aaron Packman, Northwestern University; *Physically-based Tempered Fractional-order Operators for Efficient Multiscale Simulations*
- Professor Igor Podlubny, Technical University of Košice; *Novel Matrix-Based Methods for Fractional-Order Modeling*
- Professor Karl Rohe, University of Wisconsin - Madison; *A Spectral Framework for Graph Sampling*
- Professor Chi-Wang Shu, Brown University; *Development of High Order Accurate Algorithms*
- Professor Sivaguru Sritharan, Air Force Institute of Technology; *Stochastic Analysis and Control of Compressible Flow with General Levy Noise*
- Professor Panayot Vassilevski, Portland State University; *Space-Time Discretizations Enabling Parallel-in-Time Simulations*
- Professor Gang George Yin, Wayne State University; *Networked Systems for Enhanced Adaptability: Frameworks Using Switching Diffusions, Stochastic Functional and Partial Differential Equations, and Quantum Identification and Control*

2. Short Term Innovative Research (STIR) Program. In FY15, the Division awarded four new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Susan Hagness, University of Wisconsin - Madison; *Advances in Stochastic Computational Electromagnetics Modeling Techniques*
- Professor Ryan Martin, University of Illinois - Chicago; *Variations on Bayesian Prediction and Inference*
- Professor Zhiguang Qian, University of Wisconsin - Madison; *New Sliced Space-Filling Designs Construction and Theory*
- Professor Cynthia Rudin, Massachusetts Institute of Technology (MIT); *Uncertainty Quantification for Unobserved Variables in Dynamical Systems and Optimal Experimental Design*

3. Young Investigator Program (YIP). In FY15, the Division awarded the following new YIP project to drive fundamental research in areas relevant to the current and future Army.

- Professor Jonathan Hauenstein, University of Notre Dame; *The Geometry of Multiscale Models: Identifiability, Re-parameterization, Comparisons, and Parameter Space Exploration*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY15 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Conference on Applied Statistics in Defense*; Washington, DC; 20 – 24 October 2014
- *Leading Students and Faculty to Quantitative Biology Through Active Learning*; West Palm Beach, FL; 6 January 2015
- *Microscale Ocean Biophysics*; Aspen, CO; 11 – 16 January 2015
- *Mathematics- and Computation-Enabled Materials Discovery*; College Park, MD; 20 May 2015
- *10th Conference on Bayesian Nonparametrics*; Raleigh, NC; 22 – 26 June 2015
- *Theoretical Foundations for Modeling Distributed Open Quantum Systems*; Adelphi, MD; 3 August 2015

5. Special Programs. In FY15, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded two new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Mathematical Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. Network-based Hard/soft Information Fusion. This MURI began in FY09 and was awarded to a team led by Professor Rakesh Nagi of the University at Buffalo. The goals of this research are to develop a generalized framework, mathematical techniques, and test and evaluation methods for fusion of hard and soft information in a distributed (networked) data fusion environment.

During the first four years of this effort, the MURI team developed and refined the overall system concept for human-centered information fusion and information processing architecture and developed an evolutionary test and evaluation approach that proceeds from "truthed" synthetic hard and soft data to human-in-the-loop campus based experiments. The researchers created, refined and analyzed a counter-insurgency (COIN) inspired synthetic data set ("SYNCOIN") involving both hard and soft data. The MURI team completed human-in-the-loop data collection activities involving hard sensors. The team developed a software package "Tractor" for processing text messages in multiple stages and common referencing; evaluated syntactic and semantic processing techniques and selected GATE (General Architecture for Text Engineering) for syntactic processing and FrameNet for a semantic processing database. The MURI team refined a soft data association prototype that extends the traditional hypothesis generation-hypothesis evaluation-hypothesis selection paradigm for fusion of soft data and utilizes a data graph association process.

During the final year, the MURI team made two notable transitions. The first known Hard and Soft "SYNCOIN" dataset for fusion technology and analytics development was distributed to contractors working under ARL-CISD direction and is now being employed to address CERDEC scenarios of interest. This counter insurgency dataset has about 600 natural language messages with interleaved vignettes for the development and testing of natural language processing methods, and hard sensor associable counterparts for developing semantic extraction and association technologies. This unique data sets is inspired by a Counter-Insurgency (COIN) scenario in Bagdad and contains synthetic soft (human report) data, synthetic hard (physical sensor) data, and real hard data collected using human-in-the-loop vignettes collected at a special facility in central Pennsylvania. The data are augmented by extensive "ground truth" information including, scene setter descriptions, identification and location of all events and activities, social network information, database schema, reference maps, and word cloud diagrams. In addition, the complete Hard-Soft Fusion software package and environment was delivered to ARL scientists at ARL-CISD. This includes the novel Natural Language Processing software "Tractor" with context overlay that extracts all semantically meaningful information, a best-in-class graph association engine that includes the first Map-Reduce implementation for distributed computing, and an event association engine which includes location normalization that has been competitively compared to others in the literature.

2. Measuring, Understanding, and Responding to Covert Social Networks: Passive and Active Tomography. This MURI began in FY10 and was awarded to a team led by Professor Joseph Blitzstein at Harvard University. The goal of this MURI is to develop quantitative procedures to identify, characterize and display, on the basis of externally observed data generated from passive and/or active procedures, covert social networks of asymmetric adversaries, that is, terrorist/insurgent networks.

In its first three years, the MURI team developed a framework for quantifying the fundamental limits of detectability for embedded insurgent sub-networks. This first rigorous "signal detection theory" for networks enables the computation of these performance limits within a coherent mathematical framework and the development of algorithms that approach them. This theory enables one to make trade-offs between algorithmic performance and computational requirements.

The team has encoded society+network connections (e.g., adjacency matrix with elements $\neq 0$ if tie exists) to fit a benign-background model to the encoded society+network model, fit a notional signal-plus-clutter model to partitions of the society+network model to make network signal stand out from clutter, and has begun work on statistically testing for signal presence and for use structure to localize the network in society. This is the first known rigorous signal detection theory for networks in a decision-theoretic framework.

In the fourth year of investigation, the MURI team has defined the various threads within community detection models. Within each thread, the team has developed mathematical models that are based on sociological processes which tackle subgroup detection with respect to different sociological process (language, geolocation, densities of interaction, etc.). Each of these efforts demonstrates mathematical richness, with some apparent possibility to move closer to establishing error bounds on predictions. The emphasis has remained on detection rather than general theory, has based simulation structure on real terrorist networks with quality control evaluations, and continues to emphasize the tri-thrust framework of linking social theory to mathematics, simulation and testing, and social data.

3. Structured Modeling for Low Resource Translation. This MURI began in FY10 and was awarded to a team led by Professor Jaime Carbonell at Carnegie Mellon University. The goal of this MURI is to investigate new concepts for language translation that use structured modeling approaches rather than solely statistical methods.

Whereas statistical approaches for machine translation (MT) and text analysis (TA) successfully harvest the low-hanging fruit for large data-rich languages, these approaches prove insufficient for quality MT among typologically-diverse languages and, worse-yet, are inapplicable for very low-resource languages. This research is venturing much further than just introducing syntactical structures into statistical machine translation and will turn the process on its head (*i.e.*, start with a true linguistic core and add lexical coverage and corpus-based extensions as data availability permits). This linguistic core will comprise an enriched feature representation (morphology, syntax, functional semantics), a suite of core linguistic rules that operate on these features via powerful operators (tree-to-tree transduction, adjunction, unification, etc.), and prototype MT and TA engines to evaluate their accuracy and phenomenological coverage. Contrastive linguistic analysis will identify the major translation divergences among typologically diverse languages, feeding into the MT linguistic core. Once the core is built, coverage will be broadened through additional linguist-generated rules and via Bayesian constraint learning from additional corpora and annotations as available; learning with strong linguistic priors, respecting the linguistic core, is expected to require much less data than unconstrained corpus-based statistical learning. The initial efforts are focusing primarily on African languages, such as Chichewa and Kinyarwanda (Bantu family), Tumak (an Afro-Asiatic Chadic language), Dholuo (a Nilo-Saharan language), and for even greater typological diversity, Uspanteko (a Mayan language). In addition to designing, creating, and delivering the linguistic cores for the selected languages, this research focuses on delivering a suite of methods and algorithms (*e.g.*, tree-to-tree feature-rich transducers, proactive elicitors) and their prototype software realizations.

The new powerful linguistic capabilities potentially generated by this research will enable the Army to perform rapid and principled construction of MT and TA systems for very diverse low-density/low-resource languages. This has the potential to provide the Army with new tactical capabilities for on-the-ground translation between deployed US forces and locals, especially in low density language regions. It also has the potential for new and improved capabilities for automated translation, automatic summarization, and textual analysis within the strategic intelligence communities.

4. Optimal Control of Quantum Open Systems. This MURI began in FY11 and was awarded to a team led by Professor Daniel Lidar of the University of Southern California. The goal of this MURI is to show a high degree of fundamental commonality between quantum control procedures spanning all application domains.

This research is pursuing the development of a new mathematical theory unifying quantum probability and quantum physics, and this research is developing new ideas in quantum control that are presently in their infancy. Of particular importance is perhaps the most pressing quantum control frontier: real-time coherent feedback control of non-Markovian open systems. To address this goal, the team is studying unifying features of controlled quantum phenomena. The means for achieving quantum control is generally categorized as either open-loop control, adaptive open-loop control, real-time feedback control, or coherent real-time feedback control. Despite the operational distinctions between these control categories, the researchers aim to show that there is a strong relationship between all of these approaches to control, using algebraic and topological techniques. This linkage is expected to be significant for seamlessly melding these tools together in the laboratory to draw out the best features of each method for meeting new control challenges and overcoming inevitable laboratory constraints, such as the context of proposed meso-scale laser and atomic Rb experiments.

5. Multivariate Heavy Tail Phenomena: Modeling and Diagnostics. This MURI began in FY12 and was awarded to a team led by Professor Sidney Resnick of Cornell University. The project aims to develop reliable diagnostic, inferential, and model validation tools for heavy tailed multivariate data; to generate new classes of multivariate heavy tailed models that highlight the implications of dependence and tail weight; and to apply these statistical and mathematical developments to the key application areas of network design and control, social network analysis, signal processing, network security, anomaly detection, and risk analysis.

More specifically, the researchers are investigating and developing statistical, mathematical, and software tools that will provide (i) flexible and practical representations of multidimensional heavy tail distributions that permit reliable statistical analysis and inference, allow model discovery, selection and confirmation, quantify dependence, and overcome the curse of dimensionality, (ii) heavy tailed mathematical models that can be calibrated which clearly exhibit the influence of dependence and tail weight and which are appropriate to the applied context, and (iii) exploitation of the new tools of multivariate heavy tail analysis to enable the study of social networks, packet switched networks, network design and control, and robust signal processing.

6. Associating Growth Conditions with Cellular Composition in Gram-negative Bacteria. This MURI began in FY12 and was awarded to a team led by Professor Claus Wilke of the University of Texas - Austin. The goal of this research is to develop methods to identify statistical association in multiple-input-multiple-output (MIMO) data using microbial growth and composition data.

To trace a microbe-causing disease to its source or to predict a microbe's phenotype in a given environment, it is necessary to be able to associate the conditions under which bacteria have grown with the resulting composition of the bacterial cell. However, the input and output data complexity – multiple, heterogeneous, and correlated measurements – poses an interpretational challenge, and novel methods for analyzing, integrating, and interpreting these complex MIMO data are sorely needed. The research team is thus comprised of experts in statistics, computational biology, computer science, microbiology, and biochemistry, with the goal of producing the following outcomes: (i) development of novel linear and nonlinear mathematical methods to associate bacterial cellular composition with growth conditions, (ii) identification of the types and ranges of growth conditions that lead to distinguishable cellular composition, (iii) identification of key compositional markers that are diagnostic of specific bacterial growth conditions, and (iv) assessment of model uncertainty, robustness, and computational cost. The MURI will develop capabilities in several novel areas of data analysis and statistics such as the analysis of MIMO data, the integration of side information into regression models, and inverse optimization approaches. In addition, the types of approaches developed in this project will advance DoD capabilities in bacterial forensics and enable natural outbreaks to be distinguished from intentional attacks.

7. Understanding the Skin Microbiome. This MURI began in FY14 and was awarded to a team led by Professor David Karig of the Applied Physics Lab at the Johns Hopkins University. The goal of this research is to develop a fundamental understanding of the forces shaping skin microbial communities across a range of spatial scales and to show how this understanding can be used to identify disease risk, predict disease outcomes and develop tools for disease prevention.

Human skin harbors diverse bacterial communities that vary considerably in structure between individuals and within individuals over time. The extent of this variability and its implications are not fully understood, nor is it known whether it is possible to predict what types of bacteria one is likely to find on the skin of a given individual. As a result, there are no effective tools to predict individuals more likely to acquire skin bacterial infections, then determine the efficacy of forensic analyses based on skin bacterial communities, nor to design novel strategies to limit the effective colonization of skin by pathogens. This project brings a variety of disciplines to bear on the problem: spatially explicit sampling, metagenomics, and bioinformatics will be used to characterize skin microbial communities at intermediate and large spatial scales. Molecular biology, analytical chemistry and synthetic biology will be used to probe smaller-scale processes that ultimately lead to larger-scale patterns. Ecological modeling will be used to integrate small-scale processes with large-scale patterns in order to arrive at a quantitative and predictive framework for interpreting the human skin microbiome. A series of models concentrating on four grand challenges will be built, tested and refined: (i) predicting microbiome composition based on environmental conditions, host state and microbe exposure patterns, (ii) identifying microbiome composition through volatile sensing, (iii) identifying disease risk through analysis of current state and anticipation of state changes, e.g., due to upcoming activities or events, and (iv) novel approaches for mitigating skin disease (e.g., optimal design of avoidance behavior, robustly engineered skin microbiomes). The results of this work will enable the manipulation of the skin microbiome in order to facilitate identification of allies, discourage bites of flying insects, predict skin disease, and as-yet-unimagined applications.

8. Strongly Linked Multiscale Models for Predicting Novel Functional Materials. This MURI began in FY14 and was awarded to a team led by Professor Mitch Luskin at University of Minnesota. The goal of this research is to investigate mathematical methods for strongly linking scales within the context of discovering novel functional materials.

Current research in multiscale modeling has moved little beyond weak dependence between continuum and atomistic models. In commonly-used weakly linked multiscale models, a macroscale exerts at most a homogeneous influence on a greatly separated finer scale and lacks constitutive properties, which are supplied by reaching down to the smaller scale to compute, average, and report back. Such weak multiscaling dilutes or eliminates nonlinearities and the resulting models misrepresent the observed macroscale behavior. Variabilities in microfunctional parameters not only generate uncertainty within a scale, but also propagate uncertainties between scales, both up and down, resulting in a potentially significant spread in macroscopic properties. Removing degrees of freedom from a dense system during upscaling may result in loss of information that can only be accounted for by introducing suitable random and dissipative forces that render the final mathematical formulation stochastic. This project seeks to develop a mathematical foundation for a computational framework of several strongly linked scale models for functional materials, with attendant uncertainty quantification. This will be developed within the framework of designing and discovering novel perovskite materials, mismatched alloy semiconductor materials, and 2D nanomaterials with unprecedented functional properties.

9. Fractional PDEs for Conservation Laws and Beyond: Theory, Numerics, and Applications. This MURI began in FY15 and was awarded to a team led by Professor George Karniadakis at Brown University. The goal of this research is to develop a new rigorous theoretical and computational framework enabling end-to-end fractional modeling of physical problems governed by conservation laws in large-scale simulations.

Despite significant progress over the last 50 years in simulating complex multiphysics problems using classical (integer order) partial differential equations (PDEs), many physical problems remain that cannot be adequately modeled using this approach. Examples include anomalous transport, non-Markovian behavior, and long-range interactions. Even well-known phenomena such as self-similarity, singular behavior, and decorrelation effects are not easily represented within the confines of standard calculus. This project seeks to break this deadlock by developing a new class of mathematical and computational tools based on fractional calculus, advancing the field in specific areas of computational mechanics. The fractional order may be a function of space-time or even a distribution, opening up great opportunities for modeling and simulation of multiscale and multiphysics phenomena based on a unified representation. Hence, data-driven fractional differential operators will be constructed that fit data from a particular experiment, including the effect of uncertainties, in which the fractional PDEs (FPDEs) are determined directly from the data.

The work is addressing the fundamental issues associated with the construction of fractional operators for conservation laws and related applications. An integrated framework is being pursued that proceeds from the initial data-driven problem to ultimate engineering applications. This general methodology will allow the development of new fractional physical models, testing of existing models, and assessment of numerical methods in terms of accuracy and efficiency. The integrated framework is based on a dynamic integration of five areas: (i) mathematical analysis of FPDEs; (ii) numerical approximation of FPDEs; (iii) development of fast solvers; (iv) fractional order estimation and validation, from data; and (v), prototype application problems.

C. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY15.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY15, the Division managed three new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of three Phase II contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of STTR topics published in FY14 and a list of prior-year STTR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY15, the Division managed six new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The PECASE winners for each year are typically announced by the White House at the end of the calendar year. However, the FY13-FY15 PECASE recipients had not yet been announced by the end of FY15. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY15, the Division managed six new DURIP projects, totaling $1.7 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. DARPA Biochronicity Program

The DARPA Biochronicity Program builds on studies from the DARPA Fundamental Laws of Biology (FunBio) Program. ARO co-developed the Biochronicity Program, and currently co-manages the program as a core component of the ARO Biomathematics Program's emphasis on identifying the fundamental mathematical principles of biological structure, function and development applied across different biological systems and scales. The Biochronicity program in particular seeks to achieve a fundamental understanding of the role of time in biological functions in order to be able to manage the effects of time on human physiology. For example, biological clocks are involved in regulating virtually every function of the human body, yet exactly how time contributes to cell-cycle progress, growth, metabolism, aging, and cell death is unclear. In order to understand the coordination of timing on multiple scales in the human body, the Biochronicity progr+am uses an interdisciplinary approach, involving empirical data sets, mathematical modeling, bioinformatics techniques, statistics, and data-mining, to identify common spatio-temporal instructions, or "clock signatures," regulating various physiological systems. Understanding how time regulates human biological processes should allow one to manipulate these processes so that one can for example improve trauma care on the battlefield by increasing the time available for medical treatment and surgery, as well as decrease the deleterious effects of age-related diseases and other infirmities. Along with the clear DoD relevance of the program, efforts in the Biochronicity program are leveraged by the Division's Biomathematics Program Area, Fundamental Laws of Biology Thrust.

I. DARPA Enabling Quantitative Uncertainty in Physical Systems (EQUiPS) Program

The DARPA EQUiPS Program builds on previous work in uncertainty quantification. Complex physical systems, devices, and processes important to the DoD are often poorly understood due to uncertainty in models, parameters, operating environments, and measurements. The goal of this program is to provide a rigorous mathematical framework and advanced tools for propagating and managing uncertainty in the modeling and design of complex physical and engineering systems. ARO co-manages awards within this Program. Of particular interest are systems with multi-scale coupled physics and uncertain parameters in extremely high-dimensional spaces. Novel mathematical research is being developed for dealing with the underlying high dimensionality of the space of uncertain parameters, strong multi-physics coupling, and uncertainty in the models themselves. In addition, the lack of fundamental mathematical theory for decision making and design under uncertainty for these large-scale dynamic systems is being addressed though new methods for forward and inverse modeling to scale to high-dimensional multi-scale/multi-physics systems, a quantitative understanding of uncertainties and inadequacies in the physical models themselves, and a completely new paradigm for stochastic design and decision making for complex systems. This work helps further the work done in the Division's Computational Mathematics Program Area, Mathematics of Multiscale Modeling Thrust.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Mathematical Sciences Division.

A. Semi-inner-products in Banach Spaces with Applications to Regularized Learning, Sampling, and Sparse Approximation

Professor Jun Zhang, University of Michigan, Single Investigator Award

The objective of this research is to fully develop Banach space methods for kernel-based machine learning that extend the Hilbert space framework of regularized learning. In FY15, the PI investigated Reproducing Kernel Banach Spaces (RKBS) by the semi-inner-product, developed the theory of vector-valued RKBS with applications of RKBS to manifold learning, studied frames and Riesz bases for sequence spaces, and constructed RKBS with the L1-norm known to enforce sparse solutions. The PI developed classification algorithms that are mathematically rigorous while rooted in human cognitive principles for categorization (generalization by similarity, feature selection by attention, etc.).

Based on a compressed sensing framework, the PI succeeded in constructing a low-rate spiking neuron which exploits the sparsity or compressibility present in natural signals. The model neuron belongs to the Integrate-and-Fire class; however, the PI was able to provide appropriate modifications to its dead-time to convert it into a low-rate encoder, and develop an algorithm for reconstructing/decoding the input stimulus from the low-rate spike trains. The neuron produces spikes at a firing rate proportional to the amount of information present in the signal rather than its duration. Through simulations with frequency-sparse signals, the PI demonstrated superior performance of the low-rate neuron operating at a sub-Nyquist rate, when compared with state-of-the-art neurons proposed earlier (e.g., A. Lazar's Time Encoding Machines or TEMs), which operate at and above Nyquist rates. Inspired by this research, the PI investigated Shannon's source-channel coding framework and Blahut's analysis after introducing auxiliary variables, and found that the gap of mutual information between the maximal capacity condition and the minimal rate distortion condition can be decomposed into two terms: a normalization gain (due to probability normalization) and a marginalization loss (due to probability marginalization). This analysis is based on Shannon entropy and Boltzmann-Gibbs statistics (exponential family).

Another extemporaneous direction is a formal framework to unify feature learning and generalization in a cross-table with a list of objects (in rows) and a list of features (in columns) and derive the so-called "concept lattice" - a lattice which is a partially-ordered set closed in "meet" and "join" operations. The PI was able to reformulate this existing framework as a "subset system", or a system of subsets on a set. For any subset system, it was demonstrated that, in addition to the two natural relations of subsets involved (namely, inclusion and non-zero intersection), there are two induced relations on elements of the base-set (which model *similarity* by a symmetric but non-transitive relation and *specificity* by a transitive and asymmetric pre-order relation). This allowed the PI to define "neighborhood" and "separation" in ways which extend those used in abstract topology. This provides a mathematically concise way of modeling "context" in a relational data.

B. Multivariate Heavy Tailed Statistics

Professor Sidney Resnick, Cornell University, MURI Award

The objectives of this research include generating new classes of multivariate heavy tailed models that account for implications of dependence and tail weight which can be calibrated to data, developing reliable diagnostic, inferential and model validation tools for heavy tailed multivariate data, and applying these statistical and mathematical developments to key application areas of social network analysis, network design and control, network security and anomaly detection, risk analysis, signal processing, and scheduling. Existing inference methods for heavy tail multivariate statistics are incomplete and subject to user interpretation about where to threshold and thus the inference methods are difficult to include in larger automated software routines that take the results of inference calculations as inputs. Existing methodology is typically for static, available, already collected data sets. New methods must automate the threshold selection and decide where the heavy tails begin;

they will also fetch and process data in an on-line and real-time manner. Improved graphical tools aid model selection, confirmation, and exploration, and improved inference methods and software allow more sophisticated modeling with the potential for understanding cause and effect. Similarity testing will provide the capability of classifying large, dependent datasets exhibiting multivariate heavy tail statistics into "similarity classes."

In FY15, the mathematical framework for multivariate heavy tails and the framework for strong dependence of multiple multivariate heavy tail regimes was completed by co-PI Lindskog and team. This framework presents recipes for constructing statistical families of multivariate distributions exhibiting multiple multivariate heavy tailed regimes as given by co-PIs Das and Resnick. This applies to extremal full dependence, such as asymptotically perfect risk contagion for large risks across risk classes or economic sectors, or extremal strong dependence, allowing for risks to be strongly but not perfectly extremal dependent.

Threshold selection for multivariate regular variation has developed distance correlation to decide on the threshold for independence. Measuring dependence with the Auto Distance Correlation Function has been explored for heavy tailed stationary time series such as those arising in risk analysis, and the sample autocorrelation has been found to be a misleading tool unless the time series has distinctive linear dependence. As an alternative, the Auto Distance Correlation Function is shown to be superior. The research team investigated properties of this dependence measure and developed a test of independence which can also be adapted to test for independence of two stationary time series. The limiting distribution of the test statistic has been established under suitable mixing conditions. The team has made progress in the area of negative memory and in understanding the structure of heavy tailed processes with long memory, and particularly those with negative memory where it is difficult to quantify the effect on extremes. Dimension reduction and Independent Component Analysis has been investigated and a growing, directed edge, preferential attachment model was shown to be a useful general transform technique to uncover the multivariate heavy tailed structure and should be useful for many variants of the standard model.

Sources of heavy tails have been studied and categorized in novel ways, to include generative mechanisms for power law behavior. For example, a "delusion of the weakest" can develop over a bounded parameter range where the inferior competitor can sustain an advantage over a significant but bounded period (see FIGURE 1). Where the focus is on a bivariate heavy tailed distribution with real data from images, it has been observed that the size of clusters in natural images exhibit power law behavior. The team has shown that by taking the width and the height of such clusters as 2D data that they are indeed bivariate heavy tailed. The team developed a Poisson driven stochastic differential equation model and was able to analytically calculate the tail behavior. This approach can be extended to multi-dimensional data.

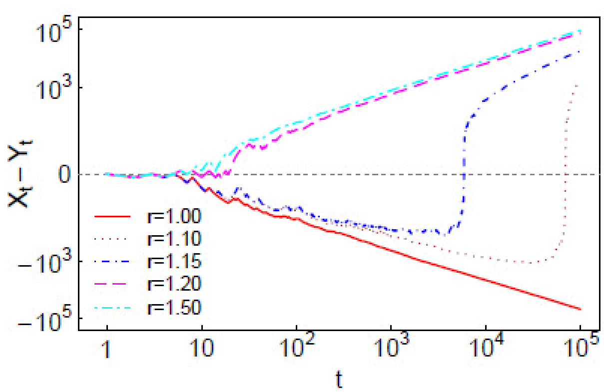

FIGURE 1

Application of heavy-tailed distributions in competition under Cumulative Advantage where advantage is marginally amplified. Emergence of "delusion of the weakest" over a bounded parameter range where the inferior competitor can sustain an advantage over a significant but bounded period.

C. Mechanisms of Bacterial Spore Germination and its Heterogeneity

Professor Peter Setlow, University of Connecticut, MURI Award

The objective of this research, co-managed with the Life Sciences Division, is to gain a detailed understanding of the germination of spores of *Bacillus* bacteria, particularly to understand the reasons for heterogeneity in germination of spores that are extremely slow to germinate, termed superdormant (SD) spores (see FIGURE 2). Dormant spores of *Bacillus* and *Clostridium* species are major agents of food spoilage and food borne disease and spores of *B. anthracis* are a major potential biowarfare agent. Thus there is great interest in methods to inactivate spores or otherwise prevent their "return to life" in germination. The fact that germinated spores are much easier to kill than dormant spores is another reason for the DoD's interest in spore germination, in particular in the causes of the extreme heterogeneity in spore germination that give rise to so-called "superdormant" spores that only germinate extremely slowly. Spores of *Bacillus* species can remain in their dormant and resistant states for years, but exposure to agents such as specific nutrients can cause spores' return to life within minutes in the process of germination.

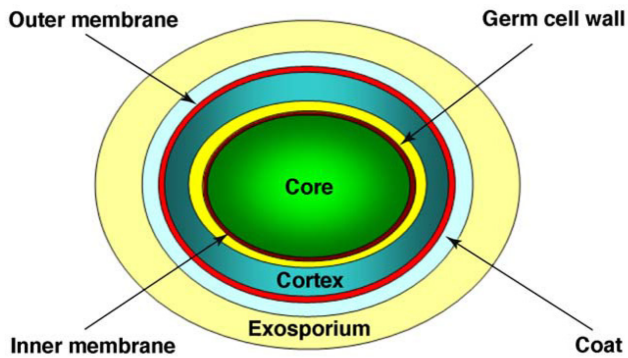

FIGURE 2

Spore structure. The various layers are not drawn to scale and there can be many sublayers in the coat and exosporium. The exosporium layer is not present in spores of all species.

By its fifth year of MURI support, this project has made significant progress in understanding how this process occurs (see FIGURE 3), discovering that this process requires a number of spore-specific proteins, most of which are in or associated with the inner spore membrane (IM). These proteins include the (i) germinant receptors (GRs) that respond to nutrient germinants, (ii) GerD protein, which is essential for GR-dependent germination, (iii) SpoVA proteins that form a channel in spores' IM through which the spore core's huge depot of dipicolinic acid is released during germination, and (iv) cortex-lytic enzymes (CLEs) that degrade the large peptidoglycan cortex layer, allowing the spore core to take up much water and swell, thus completing spore germination.

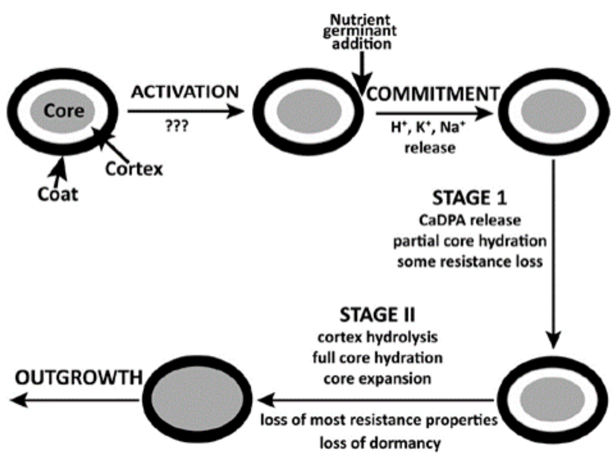

FIGURE 3

Schematic outline of nutrient germination of spores of *Bacillus* species. The precise events in the activation step are not known and are therefore denoted as question marks. The first step seen following the addition of a nutrient germinant to an activated spore is commitment, and the release of monovalent cations is associated with commitment. The germ cell wall is not shown in the figure, but this expands somehow as the cortex is hydrolyzed in stage II of germination.

In particular, mathematical modeling has been tightly coupled to experimentation in order to make progress in understanding the mechanics of bacterial spore germination. The team has developed a mathematical model that accounts for heterogeneity in both Tlag (time between nutrient germinant addition and initiation of DPA release) and commitment times. The model is built from three main mathematical components: a receptor distribution function characterizing the probability of a given spore having a particular number of GRs, a receptor activation function that determines what fraction of a spore's GRs are active given a set of external inputs (e.g., nutrient concentrations), and a germination kinetics function that specifies the number of active GRs a spore must contain in order to germinate by a given time t. This model is then used to predict the fraction of spores germinating as a function of time and germinant concentration. The parameters of the model can be obtained by fitting to experimental data on germination kinetics either from populations or individual spores. The model can also be used to fit commitment data, in which case the germination kinetics function describes the number of active GRs a spore must contain in order to commit by time t.

Germination kinetics following the quenching of germination in commitment experiments can also be used to determine how the time between commitment and Tlag varies with GR number and commitment time. Given germination data for combinations of germinants acting through different GRs, the model can be used to select or rule out plausible mechanisms of signal combination. It was found that the observed synergy between the GerA and GerB* GRs in FB10 spores can be accounted for by a model in which a common signaling intermediate accumulates at a rate proportional to the sum of the number of active GRs, but not by a model in which these GRs generate non-overlapping signals. The model can recapitulate a wide range of data generated in both wild-type and mutant spores for single and double nutrient germination, but underestimates DPA release kinetics in FB10 spore populations stimulated by L-asparagine via the GerB* GR. Recent measurements on individual FB10 spores indicate that upon stimulation with L-asparagine, many spores release DPA slowly before undergoing the rapid DPA loss characteristic of germination. DPA released in the lag period makes it appear as if spores are germinating at times when they actually are not, highlighting the importance of using single-spore data for comparison with models when mechanistic inference is the goal. Fitting of previous and newly acquired germination kinetics data with both single and double nutrient stimulation is currently underway and appears to support previous conclusions about the mechanism of synergy. This model is also in principle capable of accounting for memory effects.

Detailed knowledge of the mechanisms of spore germination and causes of superdormancy may lead to a new methodology for spore germination and thus easier spore eradication and decontamination, both of significant interest to the DoD for the purpose of preventing food spoilage. Due to this common interest, significant and ongoing collaboration has taken place between several of the labs involved in the MURI and Natick Soldier Center. This collaboration has resulted in two refereed publications, an additional paper in press, and ongoing work on the effects of heat activation on high pressure induced spore germination.

D. Local-Global Model Reduction for Large-Scale Models Integrating Systems

Professor Eduardo Gildin, Texas A&M, Single Investigator Award

The objective of this research is to study reduced-order modeling methods for multiscale processes in heterogeneous subsurface formations. In FY15, the PI investigated a new local-global multiscale model reduction framework based on system theory and on multiscale techniques for processes governed by complex systems. The concepts aim at reducing the degrees of freedom in the simulations by computing a mapping from input to output spaces, where the number of state variables and local multiscale basis are minimal. This effort involves two experienced interdisciplinary research groups from Texas A&M University and is unique in that it consolidates expertise in subsurface flow engineering and system and control theory with the formulation and analysis of multiscale methods in heterogeneous media.

In investigating systematic nonlinear complexity reduction for fast simulation of flow in heterogeneous porous media, the team has introduced, implemented, and validated two new ideas: Localized Proper Orthogonal Decomposition for the Discrete Empirical Interpolation Method (POD-DEIM), and training-free model reduction. In the case of localized POD-DEIM, the team introduced and validated a new approach to construct an efficient reduced order model for fluid flow simulation and optimization in porous media. Whereas regular POD-DEIM approximates the fine scale model with just one single reduced subspace, the localized POD and localized DEIM that are introduced in this research compute several local subspaces (see FIGURE 4). Each subspace characterizes a period of solutions in time and all together they not only are able to approximate the high fidelity model better, but also reduce the computational cost of the simulation. These two localized methods use a classification approach to find these regions in the offline computational phase. After obtaining each class, POD and DEIM are applied to construct the basis of the reduced subspace. In the online phase, at each time step, the reduced states and nonlinear functions are used to find the most representative basis for POD and DEIM without requiring fine scale information.

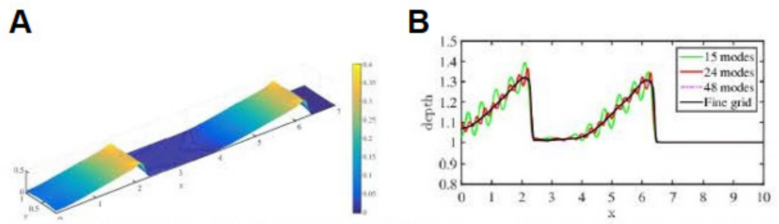

FIGURE 4

Snapshot of the fine-scale and reduced order solution for the dam-break problem. (**A**) Fine-scale solution: elevation shown with two shock fronts. (**B**) Reduced-order solution: brute force POD reduction.

The understanding developed here significantly advances the current state-of-the-art in multiscale model reductions and their applications to problems with multiple scales, parameters, and high contrast. These, in turn, will improve the ability to efficiently compute the solutions of large-scale systems that arise in the discretization of problems of linear and nonlinear flows in highly heterogeneous media.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Network-based Hard/Soft Information Fusion

Investigator: Professor Rakesh Nagi, University of Buffalo, MURI Award
Recipient: Army Research Laboratory - Computational Sciences and Information Directorate (ARL-CISD)

The objective of this research is to develop a generalized framework, mathematical techniques, and test and evaluation methods for fusion of hard and soft information in a distributed (networked) data fusion environment. Two items have been transitioned: First, the first known Hard and Soft "SYNCOIN" dataset for fusion technology and analytics development has been distributed to contractors at BAE Systems working under ARL-CISD direction. Second, the complete Hard-Soft Fusion software package and environment has been transitioned to other ARL scientists at ARL-CISD's Battlefield Information Processing Branch. This includes the novel Natural Language Processing software "Tractor" with context overlay that extracts all semantically meaningful information, a best-in-class graph association engine that includes the first Map-Reduce implementation for distributed computing, and an event association engine which includes location normalization, which has been competitively compared to others in the literature.

BAE Systems will use the SYNCOIN data set to develop new capability in context aided video-to-text information fusion in ways that support ARL-CISD requirements. ARL-CISD will use the complete Hard-Soft Fusion software package and environment to develop and expand capabilities of fusing radar moving target indicators, image intelligence, signals intelligence, video, and others sources of kinematic and classification data.

B. Studies in Structural, Stochastic and Statistical Reliability

Investigator: Professor Frank Samaniego, University of California - Davis, Single Investigator Award
Recipient: Army Evaluation Center, Reliability and Maintainability Engineering Directorate

The objective of this research is to develop structural, stochastic and statistical reliability theory for networks and engineered systems. It has made connections between these and long-standing questions in Bayesian statistical inference. The PI has transitioned statistical reliability theory algorithms to Dr. Jane Krolewsky and colleagues at the Army Evaluation Center's Reliability and Maintainability Engineering Directorate. These algorithms apply to a variety of problems in the area of reliability economics in which optimal network and system designs are sought under criterion functions which depend on both performance and cost.

The Army Evaluation Center is using these algorithms to expand their capabilities beyond reliability computations that depend on the assumption of exponentially distributed lifetimes. In particular, they are using them to address the treatment of complex systems and non-exponentially distributed component lifetimes. The algorithms implement the theory of system signatures in system reliability. The recipient is using them to address example systems whose structure or design is of a very specific type (e.g., k-out-of-n systems) and whose component's lifetimes are assumed to be non-exponentially distributed. This addresses problems in which the usual approach is impeded by one of two factors: either (1) the system's structure is sufficiently complex that obtaining an explicit representation of the system's reliability function requires advanced techniques or (2), the assumption of exponentially distributed component lifetimes does not appear defensible. It is not uncommon that analysts face both of these challenges simultaneously in particular applications.

C. Understanding Optimal Decision Making in War-Gaming Using Neurophysiological Measures
Investigator: Professor Quinn Kennedy, Naval Postgraduate School, Single Investigator Award
Recipient: U.S. Army Training and Doctrine Command (TRADOC)

The objective of this research is to investigate the role between neurophysiological indicators and optimal decision making in the context of military scenarios, as represented in human-in-the-loop wargaming simulation experiments. Specifically, an attempt was made to identify the transition from exploring the environment as a naïve decision maker to exploiting the environment as an experienced decision maker, via statistical and neurological measures.

The results of the research offer objective methods to better understand how and when an optimal decision is made and the factors that influence it. The work is coordinated with TRADOC as a possible means of refining procedures supporting more efficient learning and task accomplishment, and is also of interest to the U.S. Department of Veterans Affairs for its potential to help identify Post-traumatic Stress Disorder (PTSD) and Traumatic Brain Injury (TBI).

D. Structured Modeling for Low Resource Translation
Investigator: Professor Jaime Carbonell, CMU, MURI Award
Recipient: Defense Advanced Research Projects Agency (DARPA)

The objective of this research is to investigate new concepts for language translation that use structured modeling approaches rather than solely statistical methods. This research has gone far past just introducing syntactical structures into statistical machine translation and has turned the process on its head (i.e., starts with a true linguistic core and added lexical coverage and corpus-based extensions as data availability permits). This linguistic core comprises an enriched feature representation (morphology, syntax, functional semantics), a suite of core linguistic rules that operate on these features via powerful operators (tree-to-tree transduction, adjunction, unification, etc.), and prototype machine translation and text analysis engines to evaluate their accuracy and phenomenological coverage.

The PI has developed specific proof-of-principle cases that demonstrate success toward this objective and highlight the viability of this approach, and has transitioned these to a DARPA PM who is using these proof of principle cases and results to launch the Low Resource Languages for Emergent Incidents (LORELEI) program. In this effort, DARPA aims to dramatically advance the state of computational linguistics and human language technology to enable rapid, low-cost development of capabilities for low-resource languages. With the understanding that even with perfect translation, there would still be too much material for analysts to use effectively, LORELEI research will not be focused solely on machine translation. While LORELEI technologies may include partial or fully automated speech recognition and/or machine translation, the overall goal will not be translating foreign language material into English but providing situational awareness by identifying elements of information in foreign language and English sources, such as topics, names, events, sentiment and relationships.

To accomplish this, the LORELEI program will develop human language technology that eliminates the current reliance on huge, manually-translated, manually-transcribed or manually-annotated corpora, leveraging language-universal resources, projecting from related-language resources and fully exploiting a broad range of language-specific resources. The technologies resulting from LORELEI research will be capable of supporting situational awareness based on low-resource foreign language sources within an extremely short time frame – starting as soon as 24 hours after a new language requirement emerges. LORELEI technology is expected to be applicable to any incident in which a sudden need emerges for assimilation of information by U.S. Government entities about a region of the world where low-resource languages are frequently used in formal and/or informal media. LORELEI capabilities will be exercised to provide situational awareness based on information from any language, in support of emergent missions such as humanitarian assistance/disaster relief, peacekeeping or infectious disease response.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Structured and Collaborative Geometric Signal Models for Big Data Analysis

Professor Guillermo Sapiro, Duke University, Single Investigator Award

The objective of this research is to develop a framework for the collaborative design of signal models for ill-posed problems in signal reconstruction, classification, and identification. This will be investigated by a combination of theories from sparse modeling, Gaussian Mixture Models (GMMs), and Principal Component Analysis. Computational approaches with significantly undersampled or missing data will be considered using a collaborative compressed sensing approach and incorporation of information theory tools into sparse modeling.

It is anticipated that in FY16, the PI will solve the problem of not having an *a priori* accurate GMM, due to difficulty of obtaining training signals that match the statistics of the signals being sensed, by learning the signal model based directly on the compressive measurements of the signals without needing to resort to other signals to train the model. If successful, the likelihood estimator may be derived that maximizes the likelihood of the GMM of the underlying signals given only their linear compressive measurements, and may enable significantly better performance in signal reconstruction and identification in adverse conditions.

B. Nonlinear Stochastic PDEs: Analysis and Approximations

Professor Boris Rozovsky, Brown University, Single Investigator Award

The goal of this research is two-fold: (i) to investigate large classes of nonlinear and nonlocal stochastic PDEs and (ii), to develop related fast computational algorithms. In particular, the research addresses stochastic Navier-Stokes and Euler equations, stochastic quasi-geostrophic equations, as well as stochastic Ginzburg-Landau equations and Duffing oscillators. The research also deals with development of the necessary stochastic analysis, including generalized Malliavin calculus and generalized polynomial (L´evy) chaos.

It is anticipated that in FY16, the PI will definitely determine, either positively or negatively, whether his methods of stochastic differential equation analysis can yield a type of problem-splitting that may enable fast computational methods. Current computational methods generally require that the equations be re-solved for every data point from the (potentially multidimensional) noise distribution and then assembled into an output solution distribution. Any success in splitting could result in a tremendous decrease in computational cost.

C. Modeling Subconscious Vision

Professor Danny Forger, University of Michigan, Single Investigator Award

The objective of this research is to gain a better understanding of subconscious vision. For many years, scientists were puzzled at how many "blind" subjects could have subconscious physiological responses to light. In some subjects, light could cause pupil restriction or shift the internal daily (circadian) timekeeping system. About 10 years ago, the source of this subconscious vision was discovered; some retinal ganglion cells (RGCs) are intrinsically photosensitive (ipRGCs) even in the absence of inputs from rods or cones. A novel photo pigment, Melanopsin, which has different properties than Rhodopsin, which controls conscious vision, causes this photoreception in ipRGCs. Understanding subconscious vision will help with a better understanding of vision in general, treatments to ameliorate the condition of the blind, and better adjustment of the body's circadian clock so that our military can perform accurately 24/7.

It is anticipated that in FY16, the PI will focus on the capabilities of the ipRGC network through simulation of the network of ipRGCs by linking many copies of the ipRGC models developed earlier in the research in a spatial grid. When available, inputs from rods and cones will be added. Images such as incoming projectiles and optical illusions, will be presented to the network to determine what signals the ipRGC network can detect.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Joseph Myers
Division Chief
Program Manager, Computational Mathematics
Program Manager (Acting), Modeling of Complex Systems
Program Manager (Acting), Probability and Statistics

Dr. Virginia Pasour
Program Manager, Biomathematics

B. Directorate Scientists

Dr. Randy Zachery
Director, Information Sciences Directorate

Dr. Bruce West
Senior Scientist, Information Sciences Directorate

Ms. Anna Mandulak
Contract Support

C. Administrative Staff

Ms. Debra Brown
Directorate Secretary

Ms. Diana Pescod
Administrative Support Assistant

CHAPTER 9: MECHANICAL SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2015* is to provide information on the programs and basic research supported by ARO in fiscal year 2015 (FY15), and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Mechanical Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY15.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Mechanical Sciences Division supports research to uncover fundamental properties, principles, and processes involved in fluid flow, solid mechanics, chemically reacting flows, explosives and propellants, and the dynamics of complex systems of relevance to the Army and the DoD. More specifically, the Division supports basic research to uncover the relationships to: (i) contribute to and exploit recent developments in kinetics and reaction modeling, spray development and burning, (ii) gain an understanding of extraction and conversion of stored chemical energy, (iii) develop a fundamental understanding that spans from a material's configuration to a systems response to create revolutionary improvements through significant expansion of the mechanical design landscape used to optimizing systems, (iv) advance knowledge and understanding governing the influence of inertial, thermal, electrical, magnetic, impact, damping, and aerodynamic forces on the dynamic response of complex systems as well as improving the inherent feature set of the components (*i.e.*, mechanisms and sensing) that comprise them, (v) provide the basis for novel systems that are able to adapt to their environment for optimal performance or new functionality, and (vi) develop a fundamental understanding of the fluid dynamics underlying Army systems to enable accurate prediction methodologies and significant performance improvement, especially with regard to unsteady separation and stall and vortex dominated flows. Fundamental investigations in the mechanical sciences research program are focused in the areas of solid mechanics; complex dynamics and systems; propulsion and energetics; and fluid dynamics. Special research areas have been continued in the Army-relevant areas of rotorcraft technology, projectile/missile aerodynamics, gun propulsion, diesel propulsion, energetic material hazards, mechanics of solids, impact and penetration, smart structures, and structural dynamics.

2. Potential Applications. Research managed by the Mechanical Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by ARO research in the mechanical sciences could provide understanding that leads to insensitive munitions, tailored yield munitions, enhanced soldier and system protection, novel robotic, propulsion, and energy harvesting systems, and novel flow control systems and enhanced rotorcraft lift systems. In addition, mechanical sciences research may ultimately improve Soldier mobility and effectiveness by enabling the implementation of renewable fuel sources and a new understanding of energetic materials with improved methods for ignition, detonation, and control.

3. Coordination with Other Divisions and Agencies. The primary laboratory interactions of this Division are with the ARL Weapons and Materials Research Directorate (ARL-WMRD), ARL Vehicle Technology Directorate (ARL-VTD), ARL Sensors and Electron Devices Directorate (ARL-SEDD), the U.S. Army Corps of Engineers (USACE), and various Army Research Development and Engineering Centers (RDECs), including the Aviation and Missile RDEC (AMRDEC), Natick Soldier RDEC (NSRDEC), and the Tank-Automotive RDEC (TARDEC). The Division also facilitates the development of joint workshops and projects with Program Executive Office (PEO) Soldier and the Army Medical Research and Materiel Command (MRMC). In addition, the Division often jointly manages research through co-funded efforts with the ARO Chemical Sciences, Materials Science, Mathematical Sciences, Computing Sciences, and Life Sciences Divisions. Strong coordination is also maintained with other Government agencies, such as the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), the National Science Foundation (NSF), the National Aeronautics and Space Administration (NASA), the National Institute of Standards and Technology (NIST), and the Department of Energy (DoE). International research is also coordinated through the International Science and Technology (ITC) London and Pacific offices.

B. Program Areas

The Mechanical Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of projects. In FY15, the Division managed research within these four Program Areas: (i) Solid Mechanics, (ii) Complex Dynamics and Systems, (iii) Propulsion and Energetics, and (iv) Fluid Dynamics. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Solid Mechanics. The goal of the Solid Mechanics Program is to investigate behavior of complex material systems under broad range of lading regimes in various environments, and to develop analytical and computational methods to characterize material models and to serve as physically-based tools for the quantitative prediction, control, and optimization of Army relevant material systems subjected to extreme battlefield environments. Army systems are frequently limited by material strength and failure resistance. Solid mechanics research plays a crucial role in the development of new materials, prediction of strength, toughness and potential damage development and failure of Army material systems, structures and individual protective equipment under extreme loading conditions such as impact or blast, and prolonged normal operating conditions. Research in analytical, computational and experimental solid mechanics forms the foundation of optimization tools to enhance performance while minimizing equipment weight, and its theories provide a strong link between the underlying mechanical behavior of solids and the resulting design and functionality of actual systems resulting in reduced development cost by minimizing the need for expensive field testing and it leads to novel ideas and concepts for revolutionary capabilities.

This Program Area is divided into two research Thrusts: (i) Investigation of mechanical behavior of complex material systems, and (ii) Development of analytical, computational and experimental methods capable to utilize material models in the analysis of extreme situations leading to damage and failure development. Current program efforts utilizing advanced multiscale computational and modeling techniques enabling detailed investigations of behavior of heterogeneous solids. The goal is to extend the design envelope of current and future Army structures, to develop predictive capability based on advanced ideas and understanding of material behavior across all relevant scales, to predict continuum and localized damage and failure initiation and development as it progresses across different scales, to give reliable estimates of the material limitations and useful life.

Research in this Program Area is focused on long-term, high risk goals that strive to develop the underpinnings for revolutionary advances in military systems. It is developing the methods needed to take advantage of recent advances in new materials fabrication and investigation technology, including nanotubes, nano-crystaline solids, and bio-inspired and hierarchical polymeric- and nano-composites. As a result of the long-term vision of the program, some future applications are not yet imagined while others will lead to the creation of ultra-lightweight, high strength materials for applications such as lightweight armor.

2. Complex Dynamics and Systems. The goal of the Complex Dynamics and Systems Program Area is to develop new scientific understanding in three major research Thrusts: (i) High-dimensional Dynamical Systems, (ii) Force generation, Power and Work in Nonequilibrium Dynamical Systems, and (iii) Creating Quantitative Understanding of the Principles Underlying Biological Agility. In addition, the program has developed a set of Strategic Program Challenges (SPC) targeting questions relevant to the programmatic scientific focus areas deemed beyond the scope of single investigator awards. Current SPC topics include: (1) Energetic Versatility of Muscles: Principles and Emulation, (2) Controlling Hyperelastic Matter, (3) Theory of Morphological

Energetics, and (4) Control and Creation of Critical Dynamics.The challenges emphasize high-risk, high-reward exploratory research to create breakthroughs, push science in truly novel directions, or to support mathematical abstractions and precise physical foundations for emerging technologies deemed likely to be of significant future Army and DoD impact. SPC's are developed by the program manager in close consultation with DoD researchers and university researchers.

The Complex Dynamics and Systems Program emphasizes fundamental understanding of the dynamics, both physical and information theoretic, of nonlinear and nonconservative systems as well as innovative scientific approaches for engineering and exploiting nonlinear and nonequilibrium physical and information theoretic dynamics for a broad range of future capabilities (e.g. novel energetic and entropic transduction, agile motion, and force generation). A common theme amongst all programmatic thrust areas is that systems of interest are "open" in the thermodynamic sense (or, similarly, dissipative dynamical systems). The program seeks to understand how information, momentum, energy, and entropy is directed, flows, and transforms in nonlinear systems due to interactions with the system's surroundings or within the system itself. Research efforts are not solely limited to descriptive understanding, however. Central to the mission of the program is the additional emphasis on pushing beyond descriptive understanding toward engineering and exploiting time-varying interactions, fluctuations, inertial dynamics, phase space structures, modal interplay and other nonlinearity in novel ways to enable the generation of useful work, agile motion, and engineered energetic and entropic transformations. The programmatic strategy is to foster mathematically sophisticated, interdisciplinary, and hypothesis-driven research to elucidate classical physics and analytical methods pertinent to the foundations of a broad spectrum of Army research areas including: mobility, power and energy, sensors, lethality, and trans-disciplinary network science.

3. Propulsion and Energetics. The goal of this Program Area is to explore and exploit recent developments in kinetics and reaction modeling, spray development and burning, and current knowledge of extraction and conversion of stored chemical energy to ultimately enable higher performance propulsion systems, improved combustion models for engine design, and higher energy density materials, insensitive materials, and tailored energy release rate. Research in propulsion and energetics supports the Army's need for higher performance propulsion systems. These systems must also provide reduced logistics burden (lower fuel/propellant usage) and longer life than today's systems. Fundamental to this area is the extraction of stored chemical energy and the conversion of that energy into useful work for vehicle and projectile propulsion. In view of the high temperature and pressure environments encountered in these combustion systems, it is important to advance the current understanding of fundamental processes for the development of predictive models as well as to advance the ability to make accurate, detailed measurements for the understanding of the dominant physical processes and the validation of those models. Thus, research in this area is characterized by a focus on high pressure, high temperature combustion processes, in both gas and condensed phases, and on the peculiarities of combustion behavior in systems of Army interest. To accomplish these goals, the Propulsion and Energetics Program Area has two research Thrusts: (i) Hydrocarbon Combustion, and (ii) Energetics. The goal of the Hydrocarbon Combustion Thrust is to develop kinetic models for heavy hydrocarbon fuels, novel kinetics model reduction methods, surrogate fuel development, and research into sprays and flames, especially ignition in high pressure low temperature environments. In addition the Energetics Thrust focuses on novel material performance via materials design and development and materials characterization, and investigations (theoretical, modeling and experimental) into understanding material sensitivity (thermal and mechanical).

4. Fluid Dynamics. The vast majority of the Army weapon systems involve airborne vehicles and missile systems that are totally immersed in fluids. In turn, the performance of these weapon systems is greatly affected by the resultant forces imparted on them by the surrounding fluid. Consequently, developing highly accurate, stable, agile, and long-endurance weapon systems dictates the need for fluid dynamics research in the areas of interest to both rotorcraft vehicles and tactical missiles. In fact, the battlefield capability and tactical flight operations envisioned for the highly mobile Army of the twenty-first century can only be accomplished through scientific breakthroughs in the field of aerodynamics. Improving performances in every aspects of rotorcraft vehicle performance requires intensive fluid dynamic research in areas, such as, unsteady boundary-layer separation on the suction side of rotorcraft blades, unsteady rotor aerodynamic loads, wakes and interference aerodynamics, and computational fluid mechanics.

Ongoing research topics within this Program Area include the experimental and numerical determination of the flowfield over airfoils undergoing unsteady separation with subsequent dynamic stall, the development of micro-active flow control techniques for rotor download alleviation and dynamic stall control, and the development of advanced rotor free-wake methods to improve the predictive capability for helicopter performance, vibration, and noise. To ensure the accuracy and range of unguided gun-launched projectiles and the maneuverability and lethality of guided missiles and rockets, a thorough knowledge of the forces and moments acting during both launch and free flight is required. These objectives dictate research on shock boundary-layer interactions, compressible turbulence modeling, aft body-plume interactions, vortex shedding at high angle of attack, transonic body flows, and aerodynamic interference effects between various missile components. Examples of current studies in this subfield are the experimental study of aft body-plume-induced separation, and the use of direct numerical simulation, laser-Doppler velocimetry (LDV), and PIV techniques to investigate axisymmetric supersonic power-on/power-off base flows. Research initiatives on the aerodynamics of small unmanned aerial vehicles, both rotary wing and flapping wing, continue. Results indicate that the physics of vortex-dominated flight at low Reynolds number is quite different than that encountered for familiar high Reynolds numbers.

C. Research Investment

The total funds managed by the ARO Mechanical Sciences Division for FY15 were $13.2 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY15 ARO Core (BH57) program funding allotment for this Division was $6.6 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $2.7 million to projects managed by the Division. The Division also managed $1.0 million of Defense Advanced Research Projects Agency (DARPA) programs, $1.1 million of Congressional funds and $0.1 million provided by other Federal agencies. Finally, $1.7 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.2 million of ARO Core (BH57) funds, in addition to any funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY15 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY15 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY15, the Division awarded 19 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Amit Acharya, Carnegie Mellon University; *A Mesoscale Dislocation Mechanics Approach to Dynamically Propagating Shear Bands in Metals*
- Professor Zdenek Bazant, Northwestern University Evanston Campus; *Missile Impact with Material Comminution: New Concept - Turbulence Analogy*
- Professor Craig Dutton, University of Illinois - Urbana; *Structure and Modes of Supersonic Base Flow*
- Professor Shubhra Gangopadhyay, University of Missouri - Columbia; *Advanced Combustion Diagnostics of Al-Polymer Nanoenergetic Systems using Plasmonic and Photonic Crystal Grating Microchips*
- Professor Ari Glezer, Georgia Tech Research Corporation; *Aerodynamic Control of Coupled Body-Wake Flow Instabilities on a Free-Moving Platform*
- Professor David Gracias, Johns Hopkins University; *DNA Programmable Hydrogel Chemomechanical Actuators*
- Professor Roman Grigoriev, Georgia Tech Research Corporation; *Dynamics of turbulent Taylor-Couette flow via exact Navier-Stokes solutions*
- Professor Anette Hosoi, Massachusetts Institute of Technology (MIT); *Managing Uncertainty: Principles for Robust and Dexterous Continuum Mechanics*
- Professor Kenneth Kamrin, Massachusetts Institute of Technology (MIT); *Explaining and Exploiting the Resistive Force Theory - Toward Optimal, Flexible, Locomotor Designs*
- Professor Donald Koch, Cornell University; *Sedimentation, Orientation and Dispersal of Ramified Particles in a Turbulent Environment*
- Professor Amy Lang, University of Alabama - Tuscaloosa; *A Passive Bio-inspired Micro-adaptive Separation Control Mechanism Derived from Shark Skin*
- Professor David Lin, Washington State University; *Tuning of Musculoskeletal Mechanical Properties for Bipedal Hopping: Biological Mechanisms for Either Efficiency Versus Power*

- Professor Richard Miles, Princeton University; *Control of Static and Dynamic Stall in a Wide Range of Mach Numbers by Plasma Actuators with Combined Energy/Momentum Action*
- Professor Robert Shepherd, Cornell University; *Stretchable Capacitors that Electrically Luminesce, Sense, and Actuate for Biomimetic Coloration*
- Professor Steven Son, Purdue University; *Surface Chemistry and Combustion Behavior of Hypergolic Solid Fuels*
- Professor Stefan Thynell, Pennsylvania State University; *Experimental and Quantum Mechanics Investigations for the Development of a Liquid-phase Chemical Reaction Mechanism of RDX*
- Professor Angela Violi, University of Michigan - Ann Arbor; *Reaction Network Reconstruction for Modeling of Dynamic Pathways*
- Professor Z. Wang, University of Kansas; *A High-Order CPR Method on Overset Adaptive Cartesian and Prismatic Meshes for Rotorcraft Flow Simulations*
- Professor Kon-Well Wang, University of Michigan - Ann Arbor; *Muscle: Inspiration for a New Class of Engineered Adaptive System*

2. Short Term Innovative Research (STIR) Program. In FY15, the Division awarded six new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Sally Bane, Purdue University; *Investigation of Piezoelectric Reactives as Tunable Energetics for Advanced Munitions*
- Professor Jeffrey Bons, Ohio State University; *Synchronized Flow Control of Dynamic Stall under Coupled Pitch and Freestream*
- Professor Ronald Hanson, Stanford University; *Post-shock Sampling of Shock-heated Hydrocarbon Fuels*
- Professor Philip LeDuc, Carnegie Mellon University; *Probing Response and Future Repair of Neural Function to Impact through a Nerve Integrated Tissue on a Chip (NITC) Platform and Mechanical Approach*
- Professor Michael McAlpine, University of Minnesota - Minneapolis; *Toward Programmable Dielectric Elastomers for Actuation and Control*
- Professor Uwe Tauber, Virginia Polytechnic Institute & State University; *Toward Control of Universal Scaling in Critical Dynamics*

3. Young Investigator Program (YIP). In FY15, the Division awarded four new YIP projects to drive fundamental research in areas relevant to the current and future Army. The following PIs and corresponding organizations were recipients of the new-start YIP awards.

- Professor Caroline Genzale, Georgia Tech Research Corporation; *Spatially and Temporally Resolved Imaging of Primary Breakup in High-Pressure Fuel Sprays*
- Professor Jialiang Le, University of Minnesota - Minneapolis; *Multiscale Modeling of Probabilistic Failure of Quasibrittle Structures Under Impact*
- Professor Jesse Little, University of Arizona; *A variational method for the extraction of intermittently unstable time-dependent modes directly from system observables*
- Professor Themistoklis Sapsis, Massachusetts Institute of Technology; *Foundations of Statistical Methods for the Control of Far-from-equilibrium Driven Systems*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY15 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *2015 Laser Diagnostics in Combustion Gordon Research Conference and Gordon Research Seminar*; Waterville Valley, NH; 8-14 August 2015

5. Special Programs. In FY15, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded two new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Nanoscale Control, Computing, and Communication Far-from-Equilibrium. One MURI in this topic area began in FY13. The team is led by Professor James Crutchfield of the University of California at Davis. The objective of this MURI is to develop fundamental understanding to enable new synthetic nanoscale systems capable of behaving as information engines, performing tasks that involve the manipulation of both information and energy. Ultimately, a unified framework for understanding, designing, and implementing information-processing engines will be developed by a team of experts in information processing by dynamical systems, nonequilibrium thermodynamics, control theory, and nanoscale devices to search for and articulate the basic principles underlying the manipulation of information and energy by synthetic nanoscale systems. Theoretical predictions will be empirically validated in experimental nanoscale devices.

This research will enable new capabilities to (i) quantify the intrinsic computation in nanoscale thermodynamic systems, (ii) to produce a thermodynamic theory for control and optimization of out-of-equilibrium nanoscale processes, and (iii) to accomplish experimental validation of the resulting thermodynamic principles of optimization and control of molecular agents. The results will provide a scientific foundation for future nanoscale devices with groundbreaking capabilities, ranging from efficient computation on microscopic substrates to the generation of directed motion. In the long term, this research may enable devices that can coordinate the molecular assembly of materials and novel substrates for information processing on radically smaller and faster scales. This research may lead to a new generation of faster, cheaper, and more energy efficient computing devices capable of manipulating large-scale, complex data structures, as well as self-organizing nanoscale motors capable of interfacing with the physical world with maximum power and efficiency.

2. New Theoretical and Experimental Methods for Predicting Fundamental Mechanisms of Complex Chemical Processes. This MURI began in FY14 and was awarded to a team led by Professor Donald Thompson of the University of Missouri, Columbia. The objective of this MURI is to develop new approaches to predictive models for complex, reacting systems. It will develop supporting fundamental theory, perform supporting experiments, and validate resultant models and methods. The goal is to develop computationally efficient, predictive, accurate, robust methods to predict the molecular energy hypersurface, as well as relevant pathways and bifurcation topology for reacting coordinates.

The effort will accomplish the objectives via a comprehensive research program that will design efficient methods to predict and control the behavior of complex chemical reactions, such as combustion. Complexity is the salient challenge facing modern physical chemistry, and the proposed research will yield fundamental new methods to directly address the complexity of chemical reactions - from ab initio principles to the collective evolution of chemical populations. The research program is based on two ideas: (i) It is not necessary to describe or even know all the details, only those directly involved in the relevant pathway(s) from reactants to products, and (ii) it is essential to understand the role of fluctuations in the reaction rate, such as those that can be induced by the energetic environment and the many intermediates in combustion processes. The robust and accurate methods developed will determine the critical, emergent behaviors of complex overall reactions in non-equilibrium environments. They will accurately describe how a set of reactants undergoes sequential, branching reactions, passing through many transition states and transient species, to reach a final set of stable products. To gain an understanding of the role of fluctuations in reaction rates far from equilibrium, the researchers will focus on extracting information from the detailed dynamics of molecular species that are responsible for the fluctuations and, ultimately, the limits of traditional chemical kinetics. A synergistic approach will be undertaken for these overarching challenges that integrates the full range of rigorous fundamental theoretical methods. The specific objectives of the project leverage the complexity of kinetic phenomena, which are typically nonlinear, stochastic, multi-dimensional, strongly coupled, and can persist far from equilibrium by extreme variations in intensive properties. Some of the sub-objectives will be to: (1) Fully leverage the predictive capabilities of state-of-the-art electronic structure theory. (2) Gain a better understanding of how complex chemistry occurs at a microscopic level over wide ranges of temperature and pressure. (3) Identify and control relevant dynamical variables that can be probed experimentally. (4) Elucidate the role of statistical fluctuations in energy and matter on chemistry by analyzing the underlying nonlinear dynamics and reaction networks. (5) Design tractable theoretical and computational methods with immediate experimental links and reduced dimensionality without diminishing predictive capabilities. (6) Formulate connections among complexity theories, nonlinear dynamics, network theory, and chemistry. (7) Seek kinetic control of chemical and energetic phenomena on a macroscopic (rather than microscopic) level using nonlinear dynamics, optimal control, large deviations, and network theory.

3. **Emulating the Principles of Impulsive Biological Force Generation.** This MURI began in FY15 and was awarded to a team led by Professor Sheila Patek of Duke University. The objective of this MURI is to establish a unified theory for understanding biological and engineered impulsive systems. The MURI team will approach the objective using a thermodynamic framework linked to impulsive performance. This will require integrating mathematical analysis, tests of biological impulsive systems, and synthesis of impulsive materials and mechanisms. The thermodynamic framework consists of five phases: (1) chemical energy conversion in cellular biological systems that potentially circumvent the force-velocity tradeoffs of actin-myosin muscle mechanisms; (2) actuation tuned to spring loading through novel engineering implementations and informed by analyses of muscular and cellular thermodynamics; (3) potential energy storage through a diversity of biological materials, scales and geometries to inform synthetic elastic design; (4) rapid conversion from potential to kinetic energy (power amplification) – a defining feature of impulsive systems – through analyses of rate-dependence in biological materials/geometries, the mechanics of biological linkages and latches, and their directed synthesis into novel impulsive designs; and, (5) environment-system interactions through rigorous tests of the effects of environmental substrates and geometries, internal dissipation and reset mechanisms for repeated use and mitigation of failure due to environmental forces. This research effort will lay the foundations for scalable methods for generating forces for future actuation and energy storing structures and materials

C. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY15.

D. Small Business Technology Transfer (STTR) – New Starts

No new starts were initiated in FY15.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY15, the Division managed two new ARO (Core) HBCU/MI projects and three new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The PECASE winners for each year are typically announced by the White House at the end of the calendar year. However, the FY13-FY15 PECASE recipients had not yet been announced by the end of FY15. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY15, the Division managed seven new DURIP projects, totaling $1.6 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. DARPA Reactive Material Structures Program

The Mechanical Sciences Division serves as the agent for the DARPA-sponsored Reactive Material Structures (RMS) program. This program was initiated in FY08 with an objective to develop and demonstrate materials/material systems that can serve as reactive high strength structural materials (*i.e.*, be able to withstand high stresses and can also be controllably stimulated to produce substantial blast energy). In FY13, Phase II of the program began, which continued and expanded research efforts. Research is investigating innovative approaches that enable revolutionary advances in science, technology, and materials system performance. These approaches touch on several Mechanical Sciences Division research areas, including: rapid fracture and pulverization of the material, dispersion of the particles, and material ignition and burning, all while achieving strength, density and energy content metrics. The vision of the RMS program is to be able to replace the inert structural materials currently used in munition cases with reactive material structures that provide both structural integrity and energy within the same material system along with the ability to rapidly release the energy upon demand.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Mechanical Sciences Division.

A. Spatial Distribution of Amorphization Intensity in B4C during Rate-Dependent Indentation

Professor Ghatu Subhash, University of Florida, Single Investigator Award

At high pressures, boron carbide (B4C) experiences a localized loss of crystallinity, commonly referred to as "structural amorphization," which has been linked to a sharp decrease in its shear strength under high-velocity ballistic impact applications. This project seeks to identify the amorphization zone characteristics beneath indentation and impact loads on B4C specimens. The evolved amorphized zones under these indentations and impact sites will be compared and contrasted to identify differences in deformation and damage mechanisms as a function of indenter load, indenter velocity, impact velocity (strain rate), and projectile shape. Based on the observed size and intensity features of the amorphized zones, mechanistic models for the initiation and growth of the amorphization process will be developed. These results are expected to assist in validation of computer models for ballistic impact.

The research team conducted a fundamental study to evaluate the size and shape of the amorphized zone beneath indentation and impact surfaces of boron carbide by systematically varying the indentation load (1.7 N – 13.7 N), indentation rate (0.001/s - 5000/s), impact velocity (50-700 m/s) and projectile type (see FIGURE 1). Utilizing a novel polishing procedure to remove submicron depths of material from the loading surface and then probing each polished surface for amorphization peaks using micro Raman spectroscopy, the entire subsurface volume of the indented (and impacted) region is fully mapped to obtained the severity and spread of the amorphization zone beneath each event. These surface maps, created at various depths, are stacked together to obtain a spatial distribution of the amorphized zone beneath the loading surface. Generating such 3D maps as a function of indentation load, indentation loading rate, impact velocity, and penetrator type assists in gaining a fundamental understanding of the evolution of the amorphized zone beneath a ballistic event. Based on this information, a mechanistic-based model for the types of damage zones evolved and critical strains/pressure required for initiation of amorphization as a function of pressure and strain rate will be developed.

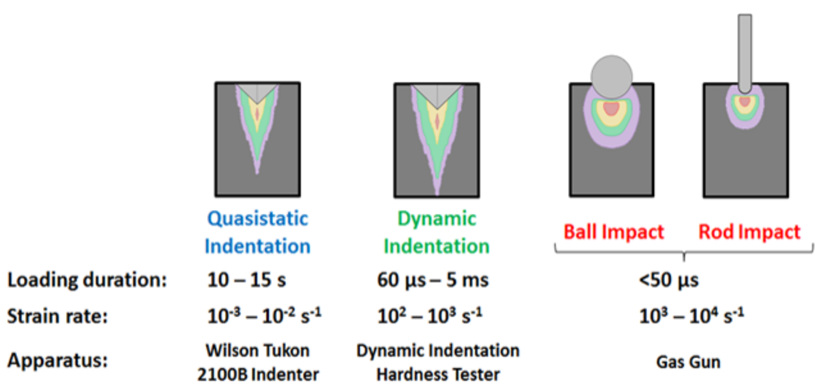

FIGURE 1

Planned experiments and schematic of the cross-sections of the resulting amorphized zones in boron carbide. The size and shape of the amorphized zone beneath indentation and impact surfaces of boron carbide were evaluated by systematically varying the indentation load (1.7 N – 13.7 N), indentation rate (0.001/s - 5000/s), impact velocity (50-700 m/s) and projectile type (ball and rod).

In FY15, the research team successfully accomplished several critical steps in the course of the project: (i) Developed a procedure for determining the depth of material removed in each polishing stage beneath the indented surface (see FIGURE 2). (ii) Created 3D maps of amorphization zones for four static loads and three dynamic indentation loads (see FIGURE 3). (iii) Developed a procedure to quantify amorphization intensity utilizing D-peak area (which corresponds to amorphization) from the Raman spectrum. (iv) Identified the variation in amorphization intensity as a function of depth beneath the indentation. Currently, 3D visualization of the damage zones which evolved due to indentation is being created utilizing optical images at various depths beneath the indentation events and a dynamic expanding cavity model is being studied to understand the evolution of various damage zones as a function of strain rate and pressure.

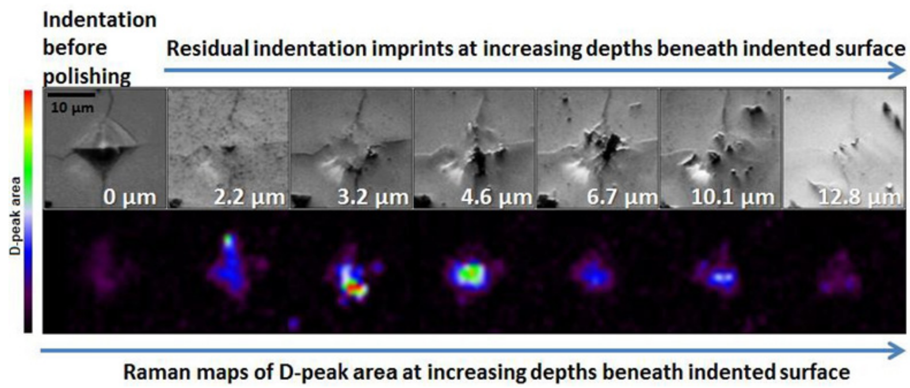

FIGURE 2

Determining the depth of material removed in each polishing stage beneath the indented surface. (**Top row**) Images of a quasistatic indentation on the surface of boron carbide and images of the polished subsurface damage at various depths. (**Bottom row**) Maps of amorphization intensity on those surfaces (generated from data obtained using Raman spectroscopy).

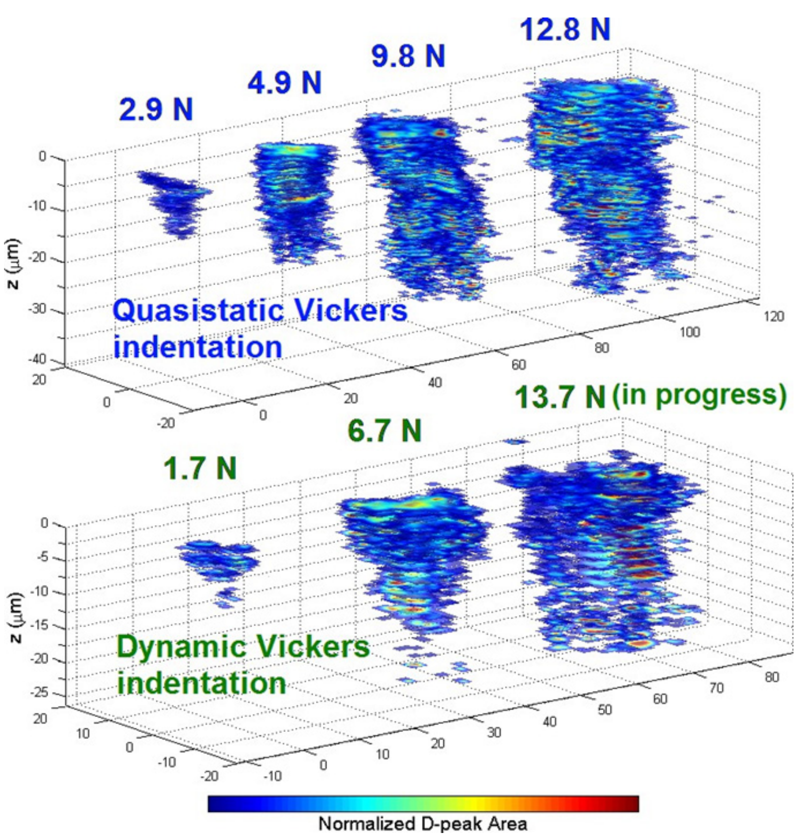

FIGURE 3

3D maps of amorphization zones for four static loads and three dynamic indentation loads. Maps of the distribution of amorphization intensity within the amorphized volumes formed by quasistatic (top row) and dynamic (bottom) Vickers indentations at various loads on boron carbide.

B. Molecular Interpenetrated Polymer Composites (MIPC) for High-Strain Rate Applications

Professor Hareesh Tippur, Auburn University, Single Investigator Award

The goals of this research are to: (i) demonstrate the feasibility of processing novel transparent interpenetrating polymer networks by combining stiff and compliant polymeric constituents and (ii) characterize their mechanical properties under high-strain rate conditions involving impact loading. On the material processing front, novel polymer systems termed Molecular Interpenetrated Polymer Composites (MIPC) comprising of two or more networks are partially interlaced at the molecular scale to produce sheet stock. Using molecular manipulations MIPCs are tailored to possess optical transparency as well as improved mechanical characteristics. High-strain rate failure characterization of MIPCs is critical for armor applications and novel techniques which can exploit their optical transparency would be of great value to characterize MIPC as well as conventional armor materials. Further, research is to develop novel, non-contact, full-field deformation measurement methods to study fracture and failure of monolithic and layered transparent sheets under stress-wave loading.

In FY15, the research team successfully demonstrated the feasibility of producing tough and highly transparent materials by means of synthesizing MIPCs. The high degree of transparency achieved in the materials was due to the successful generation of crosslinking points between the stiff and ductile polymer phases. The generation of chemical bonds between networks greatly minimizes phase separation in the polymeric system, as proven by TEM and SEM imaging and dynamic mechanical analysis (DMA). The MIPCs also showed an increase of quasi-static fracture toughness by approximately 150% when compared to PMMA. SEM imaging of fracture surfaces, however, showed no correlation between the fracture toughness and the surface area created were the crack propagated through the material. These results suggest that a different fracture mechanism govern the MIPCs.

The research team also successfully developed a new digital image correlation based optical method used in conjunction with elasto-optic principles, called the 'Digital Gradient Sensing' (DGS), to characterize mechanical properties of transparent planar solids. The method can accurately measure very small angular deflections (~10-5 radians) of light rays related to the local state-of-stress as two orthogonal in-plane stress gradients. The method has been extended to study dynamic impact on transparent sheets. The measurements during the initial stages of symmetric impact are well described by continuum based solutions. The measurements after damage initiation shed light on failure mechanisms at later stages of impact loading. DGS has been extended to study fracture mechanics of transparent acrylics under static and dynamic loading conditions. Edge notched sheets of PMMA have been studied under symmetric three-point bending and one-point impact loading conditions. Full-field stress gradient fields near mode-I cracks, before and after crack initiation, have been mapped using DGS in two orthogonal directions (normal to and along the crack) to extract stress intensity factor histories. DGS has been also used to investigate the crack growth behavior in layered transparent sheets. Bi-layered samples are prepared using acrylic adhesives to examine how a dynamically growing mode-I crack (crack speed 300-400 m/sec) in the first layer interacts with the adhesive layer. The primary interest is to examine the role of interface strength on fracture path selection in the interface and the second layer. The interface is seen to trap the crack and arrest it momentarily before triggering branched mixed-mode growth in the second layer. Optical data analysis suggests that a weaker interface dissipates more fracture energy relative to the stronger counterpart. There is also a significant crack speed reduction in the second layer (see FIGURE 4).

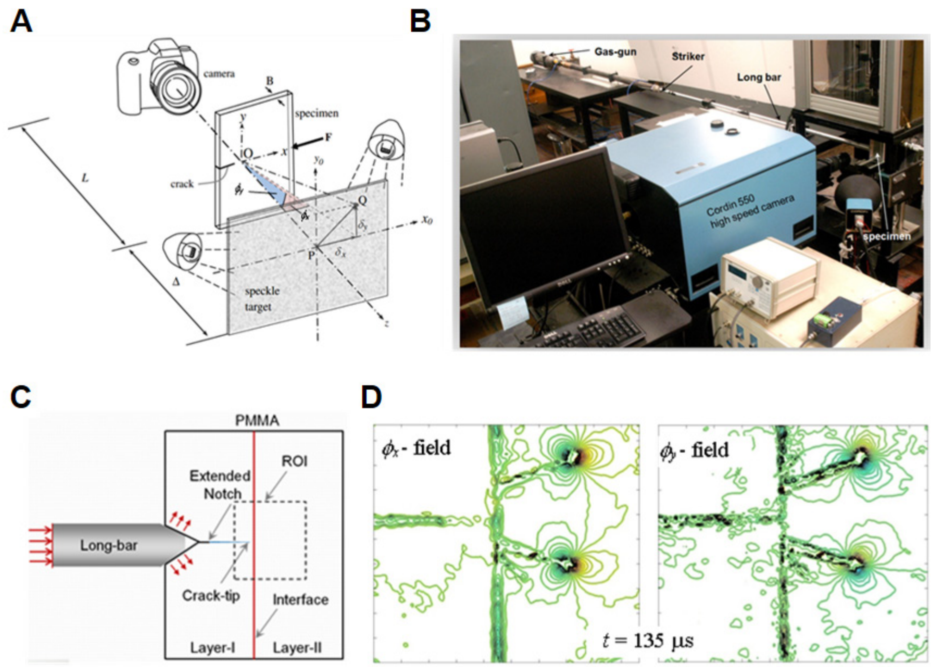

FIGURE 4

General schematic of the experiment, the image of apparatus, loading configuration, and an example of the image of processed data fields. (**A**) Schematic of the experimental setup for implementing DGS methodology to measure ϕx and ϕy in the region of interest, (**B**) photography of the DGS apparatus used to implement DGS using high-speed photography and long-bar impacting device, (**C**) schematic of the specimen configuration used to study dynamic fracture of bi-layered transparent sheets with an interface normal to crack growth direction (growth from left to right), (**D**) measured orthogonal angular deflections (proportional to in-plane stress gradients) at a time instant when the crack is propagating as a branched mixed-mode crack in layer-2.

C. Exploration of Soft-Matter Phase Transitions in Fire-Ant Aggregations

Professor David Hu, Georgia Institute of Technology, Single Investigator Award

The goal of this research is to develop a program to discover adaptability principles of fire ants, Solenopsis invicta, under diverse conditions. This work will build on the PI's previous work on fire ants to discover principles of shelter construction, adaptation to vibration, internal dynamics of aggregations, and responses to external forces. The program will be composed of four research thrusts, each of which can operate separately but will ultimately interact: instrumentation development, biological studies, physical modeling and material properties characterization. These will advance biomechanics, robotics and active materials research. While much headway has been made into the principles of swarm behavior such as in bird flocks and schools of fish, less is understood about how systems can build permanent structures and adapt to stressful environments. There is a need for simple modular robots that can work together for reconnaissance and that can maintain structures in unknown environments. This study shows how fire ants are able to collectively change their group structures to survive using decentralized control. The principles found in this study will help guide in design of modular robots as well as the algorithms to guide them in building in dynamic environments.

This program had a significant research contribution in FY15. Solenopsis invicta link their bodies together to form a variety of structures, including rafts, towers and bridges. Remarkably, these ant aggregations exhibit behaviors that are inherently both liquid-like and solid-like: they drip and spread, like simple liquids, but also withstand applied loads and adopt defining shapes, like solid materials. Since the ants are living organisms that are out-of-equilibrium, constantly transforming chemical energy into work, fire ant aggregations can be regarded as an active material. This denomination has increasingly been used to describe a wide variety of natural and synthetic materials, including flocks of birds or fishes, active liquid crystalline materials and cellular assemblies; these are regarded as predominantly liquid-like, if the building blocks are unable to link and rather are always separated from one another, and predominantly solid-like, if the building blocks are in direct contact with each other and mostly locked in position. In contrast, data indicates that fire ant aggregations are clearly viscoelastic, with equal elastic and viscous contributions. The researchers found that the elastic and viscous moduli, measured in the linear regime using oscillatory rheology, are identical in magnitude over the spanned frequency range, emphasizing the lack of a dominant structural relaxation (see FIGURE 5). Additionally, when deformed beyond the linear regime, fire ant aggregations flow and exhibit a marked shear thinning behavior, with a stress load that is comparable to the maximum load the aggregation can withstand before individual ants are torn apart. The rich behavior exhibited by this new class of active material can not only provide new insights into how systems that are out-of-equilibrium can collectively respond to emulate the behavior of inanimate fluids and solids, but it can potentially illuminate what could in the future be achieved in the fields of modular, micro- and nano-scale robotics.

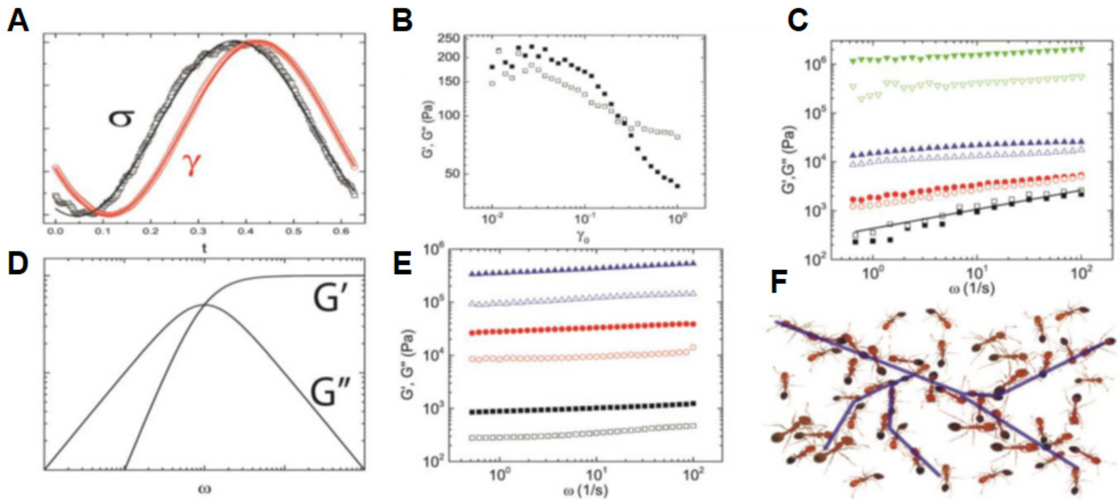

FIGURE 5

Viscoelasticity of fire ant aggregations. (A) Waveforms of the applied strain and measured stress from the linear regime of live ants at a density of 0.34g/cm3 with corresponding harmonic fits. From the fits of the raw waveforms researchers can determine the elastic, G', and viscous, G", shear moduli. (B) G' (closed) and G" (open) as a function of strain amplitude. The cutoff at low strain amplitude was determined by the minimum torque limit in the experiments. (C) Frequency sweep in the linear regime for live ants. As the ant density is increased G' progressively becomes larger than G" and becomes more frequency independent. (D) Frequency dependence of G' and G". The main feature is the existence of a crossover point between G' and G", indicating there is a single relaxation time for the material. The behavior seen for ant aggregations dramatically differs from the expectations of a viscoelastic Maxwell model, indicating that these materials do not have a single relaxation time. (E) Frequency sweeps of dead ants in the linear regime for three different ant densities. For all three densities G' is larger than G" over the entire frequency range and exhibits little frequency dependence. This indicates the elastic nature of the dead ant aggregations. (F) Schematic of a live ant aggregation. The connectivity between ants results in the elastic nature of the aggregation, while the break-up of contacts and ant rearrangements results in the viscous nature of the aggregation. The formation and breaking of these inter-ant contacts is what results in the observed viscoelastic behavior.

D. Incipient Soot Formation in Rich Partially Premixed Flames under High-Pressure Conditions

Professor Alessandro Gomez, Yale University, Single Investigator Award

The objective of this research is to examine the onset of soot in counterflow laminar systems operated under (partial) premixed burning in a high-pressure (5 MPa) regime of relevance to compression ignition (CI) engines. The ultimate goals is to shed light on the particle inception process, the most critical and relatively unclear step in soot formation. This entails the transition from gas phase precursors to nanometric solid particles. An additional goal is to examine the transition from flame to the Low Temperature Combustion (LTC) regime, as a function of stoichiometry, dilution level and feed stream composition. The approach to achieving the objectives will be to optimize gas sampling with the minimization of probe intrusiveness at high pressures, analyze the gas by gas chromatography and mass spectrometry, sample nascent soot particles, if present, with sufficient spatial resolution even for the expectedly thin flames at high pressures, and compare the developed database with chemical kinetic modeling. In the first year, the researchers will pursue the upgrade of an existing pressurized combustor with the incorporation of feed stream preheating to ensure operation up to 5 MPa. They will investigate spatially resolved thermophoretic deposition with variation of substrate size and materials and develop complementary ensemble laser light scattering/extinction techniques.

In FY15 the researchers investigated an incipiently sooting ethylene diffusion flame that morphed into a double (premixed/diffusion) flame structure when oxygen was added on the fuel side at constant peak temperature and stoichiometric mixture fraction. They performed temperature measurements using fine thermocouples and thin filament pyrometry, as well as gas sampling through a quartz microprobe followed by GC-MS analysis. As a result, a database was developed with the measurements of primary reactants, products and intermediates, including critical soot precursors up to 3-ring aromatics. This has been compared with the results of laminar flame computations using two chemical mechanisms. At equivalence ratio Φ=6.5 and Φ=5.0, the dual flame sandwiches an incipiently sooting layer and, as the equivalence ratio decreases, soot formation increases- a trend that is qualitatively observed also at Φ=3 (see FIGURE 6). It was found that the premixed component of the flames and the diffusion flame one are both thermally and chemically coupled, with the premixed flame fueling the diffusion flame with CO and H_2. As the equivalence ratio decreases, the post flame region on the premixed side contributes more and more to the production of critical soot precursors (e.g., C_2H_2 and C_6H_6). This contradicts what is typically observed in purely premixed flames and suggests a peculiar nature of these aerodynamically stabilized partially premixed flames. It can be explained in part because of the increased separation of the two flame components, with the oxidative ability of the diffusion flame reduced at low Φ, in part as a result of changes in the temperature-time history downstream of the premixed flame. Comparisons with computational results showed good agreement for major species and some soot precursors such as benzene and acetylene, despite mismatches in some critical intermediates. If benzene is considered as a soot surrogate, the computational comparison between partially premixed flames and their purely premixed strained counterparts shows that the two sets of flames behave likewise in terms of dependency of sooting tendency on equivalence ratio and peak temperature. Furthermore, partially premixed flames, probably as a result of the back diffusion of key radicals such as H and OH from the diffusion flame component, have lower tendency to soot as compared to purely premixed ones.

FIGURE 6

Investigation of incipiently sooting ethylene diffusion flame that morphed into a double (premixed/diffusion) flame structure. Image of a Φ=5 partially premixed flame at Tmax=2000 K showing a double (two-stage) flame structure, with a premixed flame at the bottom, a diffusion flame at the top and a soot layer in between. The orange line superimposed on the images highlights the position of the Gas Stagnation Plane (GSP).

To characterize the soot layer, the researchers explored thermophoretic sampling that is particle-size independent in the high Knudsen number regime. The researchers identified that the use of much thicker probes such as 140 um SiC wire that were pre-treated in lean flames to clean the surface properly before collecting soot. Scanning Electron (SEM) and Helium Ion Microcopy (HIM) images of several samples were analyzed in a semi-automated fashion to infer the particle size distribution function (PSDF). The soot sample size and size distribution is found to be virtually invariant with the probe residence time in the flame, which implies that surface kinetics and/or condensation growth are not an issue. For diameters larger than 4-5nm, the measured PSDFs can be well approximated by a lognormal distribution. Neither microscopy technique is able to identify a smaller mode of the distribution, but the HIM revealed a more extensive particle coverage as compared to SEM analysis. Examining the samples at grazing incidence with respect to the opaque substrate, using Transmission Electron Microscopy (TEM), revealed the presence of particles as small as 2 nm, and it was not possible to distinguish even smaller particles because of the substrate surface irregularities. The smallest particles have an increasingly smaller contact angle with the substrate with decreasing size as opposed to the spherical shape of particle larger than 7 nm.

The researchers compared the soot data collected with different techniques for the same burner-stabilized premixed flame (see FIGURE 7). The comparison highlights limits of each diagnostic. The PSDFs at HAB=12.5mm are superimposed to each other for diameters larger than 9nm whereas the thermophoretic sampling technique increasingly underestimates the particle number concentration for smaller sizes as a consequence of the SEM decreasing resolution in this size range. No particles were thermophoretically collected at HAB=10mm, consistent with the DMA finding that most of the particles are smaller than 3 nm when the appropriate DR/Δt is used, i.e. lower than the SEM detection limit.

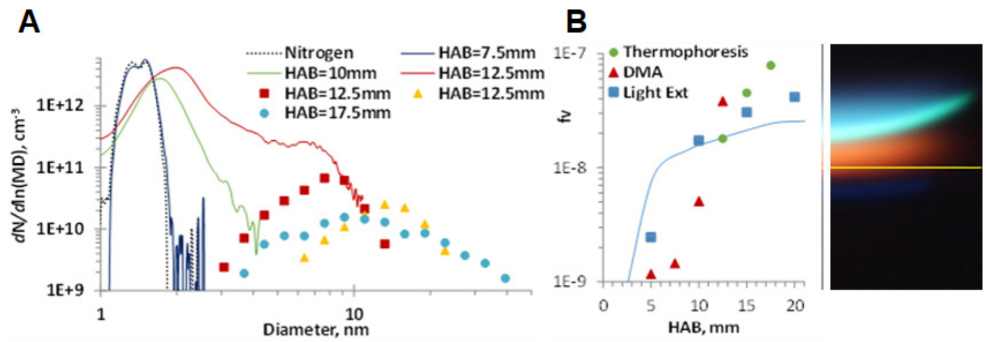

FIGURE 7

Comparing DMA and thermophoretic sampling data. (**A**) Measured soot PSDFs at several HABs using DMA (continuous lines) or thermophoretic sampling (symbols). (**B**) soot volume fraction (continuous line from data from ISFW). Data were compared with those available online from the ISFW website, shown as a continuous blue line. The data are self-consistent: soot volume fractions are slightly underestimated by the DMA techniques at HAB below 7.5mm that is where the average particles sizes are below 2 nm.

E. Rational Engineering of Reactive Nanolaminates for Tunable Ignition and Power
Professors Jon-Paul Maria and Donald Brenner, North Carolina State University, Single Investigator Award

The objective of the proposed research effort is a collaborative experimental-computational investigation of reactive nanolaminate structures identified as attractive new energetic materials with potential for tunable yield. The material combinations proposed belong to a family of metal/metal oxide nanolaminates that are thermodynamically predisposed to the rapid release of chemical energy via oxygen exchange. The energetic systems to be studied are subject to physical experiments, computational modeling, and study via external collaborations with other researchers in the area. The experimental effort is designed to isolate variables that are likely to influence mass transport in reactive laminates and to identify the material combinations and physical dimensions that enable tailored yield. The Maria Group prepares all multilayers with a two-source magnetron sputtering system with the proven capability to synthesize multilayer thin films with flat interfaces and well controlled and reproducible thickness profiles. The Maria Group has a Netzsch DTA/TGA dedicated to this nanolaminates program and can be used to identify quantitatively activation energies for oxygen exchange, and identify semi-quantitatively the energies released. For the computational effort, the materials will be considered as source and sink materials for oxygen transport. The point defect enthalpies in source and sink materials will be characterized using first principles density functional theory (DFT). These methods are transferable and will provide a robust method to handle the mixed bonding in this system. The Brenner Group conducts the computational work. The external collaboration is conducted with the Dlott (University of Illinois Urbana-Champaign) Group and the Zachariah (University of Maryland) Group.

In FY15, several accomplishments were achieved. First, laser driven flyer plate shock impact work was conducted by the Dlott group on Zr/CuO thin film samples developed by the Maria Group. The Zr/CuO was deposited on masked glass with varying bilayer thicknesses from 1 μm down to 400 nm, overall sample volume and thickness was kept constant at 1 μm. The samples correspond exactly to the samples tested at slow heating rates in previous tests. The samples were shot with Al flyer plates at a set of velocities and optical emission versus time data was collected from the back side of the thin-films (see Figure 8). As expected as the interfacial density increased (and the diffusion distance decreased) the required flyer plate velocity needed to initiate exothermic oxygen exchange decreased from 1120 meters per second for the one bilayer system, to 940 m/s for the two bilayer system, and to 750 m/s for the three bilayer system. Note that this data was first reported in 2014, since then, the same experiment was repeated several times to ensure reproducibility and to generate a self-consistent understanding.

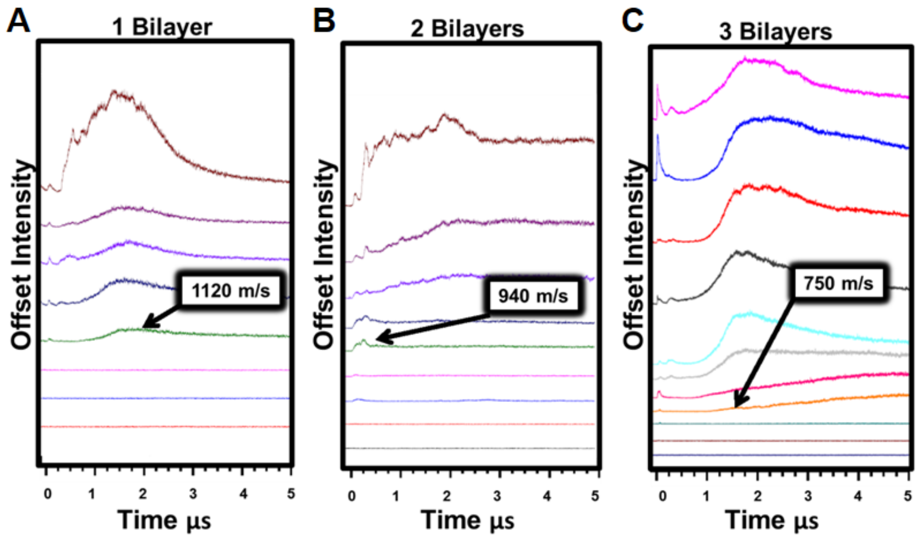

FIGURE 8

Results of bilayer thickness variation experiment where each trace represents a different flyer plate velocity incident on the sample. Intenstiy vs time data where each trace represents the optical emission spectrum of increasing flyer plate velocities for (A) Zr/CuO 1bilayer sample, (B) Zr/CuO 2 bilayer sample, and (C) Zr/CuO 3 bilayer sample

Additionally, in the collaboratory effort the Zachariah Group, the researchers demonstrated the ability to test thin-film thermite with heating rates on the order of 105 Kelvin per second. The thin platinum wires that are used in the fast thermal characterization process are 75 µm in diameter. PVD was used to obtain a conformal thin-film thermite coating around these wires that is uniform over the entire length. Aluminum and copper oxide were deposited on a rotating platinum wire with known deposition duration. The aluminum layer was deposited first followed by the oxide. During the thin-film thermite deposition each sample had a total thickness of 1800 nm and the number of bilayers was varied from 1 to 12 (see FIGURE 9).

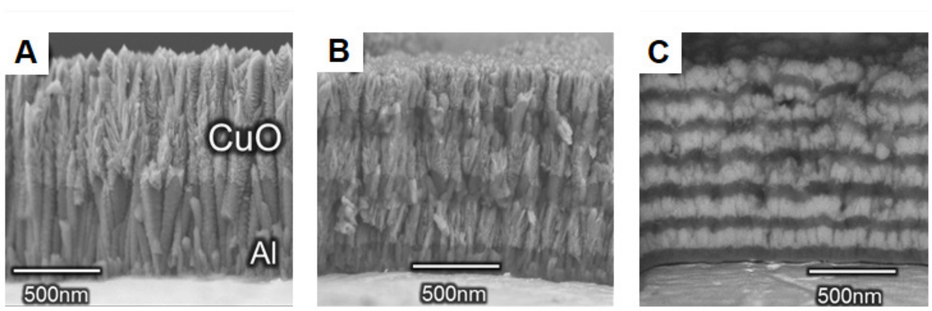

FIGURE 9

Cross-section SEM micrographs of Al/CuO nanolaminate. Bilayer numbers varied from (A) 1 bilayer, (B) 3 bilayers, and (C) 6 bilayers.

Experiments using a temperature ramp of roughly 4 x 10^5 K/s were conducted. During the rapid anneal high-speed camera images taken 67,000 times a second from a Phantom v12.0. From the analysis, accurate ignition temperatures can be ascertained within 50 K. During the high-speed anneal the chemical identification of the reaction products is analyzed every 100 µs via time of flight mass spectroscopy. Collectively this experimental procedure allows for the determination of ignition temperature and the characterization of the chemical products ejected from the platinum wire for nano laminate thermite samples. Using image analysis, the point of ignition is determined for all of the samples for various ignition temperature and relative geometric characteristics. The data show a clear trend of decreasing ignition temperature with the increase in interfacial density.

Further analysis of the emission from these thermite thin films on platinum wires via integrated intensity from the high-speed video frames show that in addition to lower ignition temperature the samples with the higher number of bilayers also displayed an increase in reactivity. Namely, the integrated intensity from these reactions, which can be correlated to a hotter reaction, grew as a number of interfaces increased.

This increased reactivity was also observed in the time of flight mass spectroscopy. Three bilayers displayed very little product particulate signal during the temperature ramp, until about 900 °C where a large oxygen signal is noticed. In the 6 bilayer sample, numerous products are detected at around 500 °C. It is speculated that in the three bilayer samples, CuO is reduced prior to ignition, while in the 6 bilayer sample, the oxygen exchange reaction occurs due to a high interface density.

In summary, thin Pt wires were coated with thin film thermite reactants pairing aluminum with cupric oxide. Temperature jump coupled with mass spectroscopy experiments were done on the thin laminate films with a variation of interfacial density and reaction distance while the total volume of reactants held constant. The temperatures of ignition were determined to decrease as a function of decreasing bilayer thickness. A simple ignition model was devised by the Zachariah Group to estimate the activation energy of the reaction process that was found to be lower than any reported values for the activation energy of diffusion through alumina.

F. Detailed Measurements of the Aeroelastic Response of a Rigid Coaxial Rotor in Hover

Professor Jayant Sirohi, The University of Texas at Austin, Single Investigator Award

The objective of this research is to gain fundamental understanding of the aeromechanics of coaxial counter-rotating (CCR) rotor systems during hover through a combination of experimental and physics-based analysis methods. A DURIP-supported CCR hover facility, with a Mach-scaled rotor system, has been installed at The University of Texas at Austin (see FIGURE 10). Experimental investigations are currently underway to measure the static and dynamic structural response of the CCR system at hover conditions. CCR rotor systems are under consideration as enablers for next-generation rotorcraft, which require forward speeds in excess of the current capabilities of single main rotor systems. In spite of demonstrated capabilities of CCR prototypes, little experimental flowfield data exists that allows fundamental understanding of the velocity distribution in the rotor system wake at hover or in forward flight. This understanding is crucial to future aerodynamic performance.

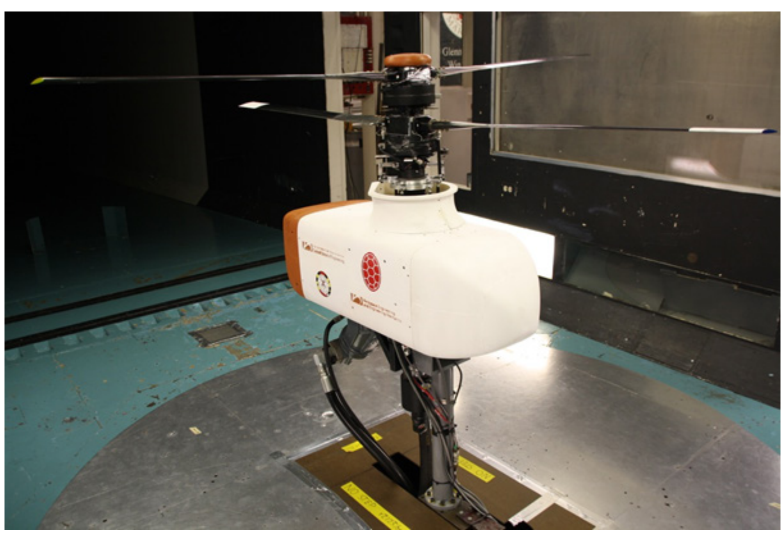

FIGURE 10

Coaxial counter-rotating (CCR) rotor system test stand installed in the University of Maryland tunnel for forward-flight testing. The CCR rotor system has load cells and other sensors to monitor the performance of each rotor, as well as their combined effect.

In FY15, dynamic calibration of the hub-mounted load cells was completed, which allowed the researchers to account for significant non-linearity associated with complex loadings (combined thrust and loading moments). Blade deformations were measured using Digital Image Correlation (DIC) techniques, revealing that deformation of the lower rotor in the coaxial configuration is less than an identical single rotor (see FIGURE 11). The DIC system is also capable of quantitatively identifying blade pitch angle and tip bending deflection. Preliminary testing of the CCR rotor system in forward flight has also been conducted at University of Maryland and will continue in summer FY16.

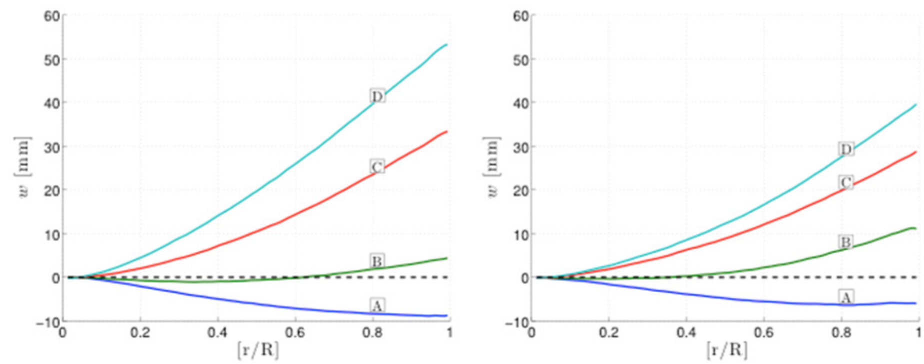

FIGURE 11

Rotor blade bending deformation. (Left) Isolated single rotor and (Right) lower rotor of the CCR rotor system. Cases A, B, C, D correspond to the same blade loadings for each case, with curve A representing the lowest loading and curve D representing the highest blade loading. At low blade loading, centrifugal force caused downward flap bending.

G. Nonlinear Aeroelastic Analysis of Two- and Three-Dimensional Dynamic Stall

Professor Marilyn Smith, Georgia Institute of Technology, Single Investigator Award

The objective of this research is to investigate the complicated dynamic fluid-structure interactions that can occur when aerodynamic surfaces experience dynamic stall. Dynamic stall occurs when an aerodynamic surface experiences rapid changes in angle of attack, leading to unsteady separation and reattachment of the boundary layer. Advanced computational fluid dynamics techniques, using hybrid Reynolds Averaged Navier-Stokes/Large Eddy Simulation formulations, are used to investigate the flow physics. Reduced order models are subsequently developed to allow rapid calculation of aerodynamic performance for use in design and in rotorcraft flight simulation.

In FY15, several advances in computational capabilities were made. During forward flight of a helicopter, the retreating blade experiences flow velocities with reversed direction. This reverse flow regime is also susceptible to dynamic stall which can be severely limiting to aerodynamic performance. Recent accomplishments include the successful blind correlation of computational results with experimental measurements, along with identification and characterization of static and dynamic stall stages in the reverse flow regime (see FIGURE 12).

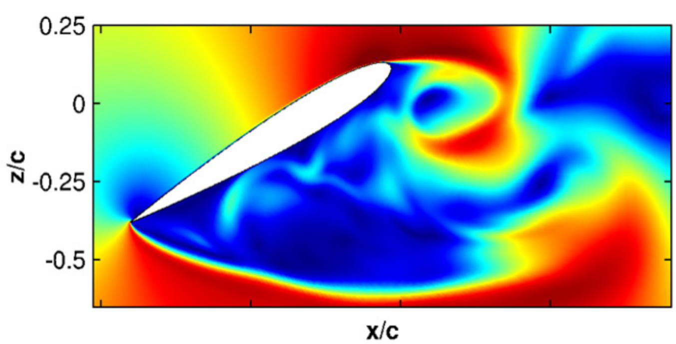

FIGURE 12

Snapshot of massive boundary layer separation in the reverse flow deep stall regime. Angle of attack variation is greater than 12 degrees and chord Reynolds number is 1.1(105).

In addition, examination of the predicted flow physics allowed for the development of improved algorithms, which enhance the ability to capture phasing between aerodynamic surface position and flow-induced forces and allow a computational speed increase of more than 70%. Reduced order models developed from understanding gained as a result of the computations have produced results well-correlated with experimentally measured performance of NACA 0012 and VR-12 airfoil shapes. The reduced order models include effects of secondary stall peaks, unsteady free-stream, yaw, three-dimensional inflow and radial coupling effects and are capable of giving reasonably accurate performance data in real-time (see FIGURE 13).

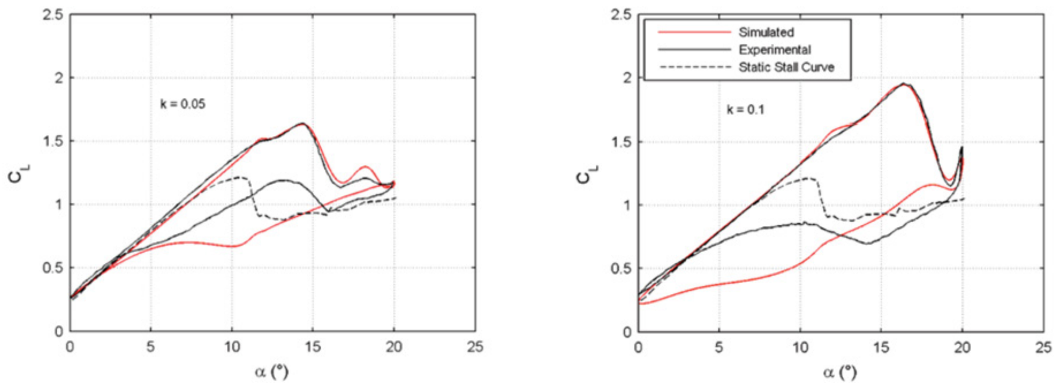

FIGURE 13

Lift coefficient on the VR-12 airfoil section as predicted by reduced order dynamic stall model. Comparison (red) with experimental results (black) and static stall performance (dashed) for reduced frequency 0.05 (left) and 0.1 (right) at Mach 0.4.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Scaling Relationships for Mesoscale Modeling of Dynamic Failure in Titanium and Titanium Alloys

Investigator: Professor Avinash Dongare, University of Connecticut, Single Investigator Award
Recipients: ARL Computational and Information Sciences Directorate (ARL-CISD)

The goal of the research project is to develop microstructure-failure-strength relationships at mesoscales in lightweight metallic systems under dynamic loading conditions and bridge the gap between atomistic and continuum simulations. To achieve this goal, a novel mesoscale modeling method is developed by the PI that extends the time and length scale capabilities of MD simulations in the mesoscales. The mesoscale behavior is enabled by choosing representative atoms to model the dynamics of several atoms in an atomic scale microstructure. Scaling relationships are used to retain the energetics and the atomic scale degrees of freedom for these representative atoms as well as the missing atoms. To achieve this goal, a novel mesoscale modeling method called quasi-coarse-grained dynamics (QCGD) is developed by the PI that extends the time and length scale capabilities of MD simulations in the mesoscales. The mesoscale behavior is enabled by choosing representative atoms to model the dynamics of several atoms in an atomic scale microstructure. Scaling relationships are used based on the atomic scale interatomic potentials to retain the energetics and the atomic scale degrees of freedom for these representative atoms as well as the missing atoms. This scaling allows larger size systems and improved time-steps for simulations and is thus able to extend the capabilities of MD simulations to model materials behavior at mesoscales. The QCGD method can retain the atomic scale degrees of freedom for representative atoms that define the energetics of the QCG system and implicitly retain the thermodynamic behavior and the mechanical behavior as predicted by MD simulations.

The project has currently investigated the deformation and failure response of single crystal and nano-crystalline systems of pure titanium, aluminum and magnesium under dynamic loading conditions using molecular dynamics (MD) simulations. These simulations are aimed to understand the fundamental micromechanisms related to the deformation, phase transformation, and failure at the atomic scale resolution during shock wave propagation. The code/data transitioned to ARL-CISD where the code is being used by the ARL researchers for MD simulations of materials relevant to the Army to model relationship between material atomic structure and the mechanical properties under high rate dynamic loading conditions.

B. Multiscale Adaptive Large Eddy Simulation and Direct Numerical Simulation of Turbulent-Chemistry Interaction of Stratified Charge Fuel Ignition

Investigator: Professor Yiquang Ju, Princeton University, Single Investigator Award
Recipient: CD-Adapco

The objective of this research is to address the limitation of today's turbulent combustion modeling capabilities and to develop a new high fidelity Multiscale, chemistry and physics Adaptive, Large Eddy Simulation and Direct Numerical Simulation (MA-LES/DNS) method to model stratified diesel combustion of jet and diesel surrogate fuels. This has led to the development of a Correlated Dynamic Adaptive Chemistry and Transport (CO-DACT) method which significantly improves computational efficiency of transport properties over previous (CO-DAC) methods by correlating key transport parameters across cell groups of time and space. This leads to gains in computational efficiency of over two orders of magnitude.

In FY15, the researchers began collaboration with CD-Adapco to transition and incorporate the method incorporation into its Star-CD and Star-CCM CFD codes for reacting flow systems. This will allow significantly more detailed and more accurate chemistry calculations to be conducted on reacting flows with no impact to computational cost.

C. Novel Framework for Ground Vehicle Mobility Prediction and Autonomous Movement
Investigator: Professor Karl Iagnemma, Massachusetts Institute of Technology, Single Investigator Award
Recipients: Tank and Automotive Research, Development and Engineering Center (TARDEC); Engineer Research and Development Center (ERDC)

The objective of the research is to investigate methods for stochastic vehicle mobility prediction over large-scale terrain regions, for eventual integration into a next-generation NATO-reference mobility model (NRMM) framework. The PI, in collaboration with Army scientists at ERDC and TARDEC, developed and experimentally validated a novel framework for (possibly autonomous) ground vehicle mobility prediction over large spatial regions. The mobility prediction framework uses geostatistical methods to create a terrain model and then rigorously evaluates vehicle performance by considering (1) uncertainty in terrain elevation, (2) new data on deformable soil properties, and (3) novel physical models of vehicle-terrain interaction phenomena. Importantly, the framework features global path planning rather than local path planning (i.e. planning in the close vicinity of the vehicle), providing new capabilities for data-supported movement decisions over large spatial regions beyond simple go/no-go decisions. This framework could (1) provide Army decision-makers with a comprehensive and reliable analysis of the mobility capabilities of their vehicles before attempting a mission, (2) enable high-fidelity simulations to improve design and operations of a large class of vehicles, (3) increase capabilities of vehicles by integrating with Graphical Information Systems, and (4) form part of a next-generation NATO-reference mobility modeling tool.

D. Intrinsically Efficient and Accurate Viscous Simulations via Hyperbolic Navier-Stokes Systems
Investigator: Dr. Hiroaki Nishikawa, National Institute of Aerospace, Single Investigator Award
Recipient: National Aeronautics and Space Administration (NASA)

The objective of this research was to generate a Reynolds-Averaged Navier-Stokes solver based on a novel first-order hyperbolic system method. Such a scheme has been developed and has shown success in the ability to compute 3rd order accurate solutions faster than traditional second order methods. Additionally, high order accuracy calculations of gradient quantities are possible on irregular grids; this overcomes a substantial hurdle to generating spatial discretization on complex geometries while maintaining accuracy and efficiency. Addition of an artificial hyperbolic diffusion to the equations (on the order of machine accuracy) provides a necessary symmetry breaking that allows higher-order accurate computations of gradients, necessary for computation of vorticity and other important quantities.

In FY15, Dr. Nishikawa forged a collaboration with researchers at NASA Langley, demonstrating the residual-distribution method for arbitrary triangular grids for model advection-diffusion problems. This permitted the demonstration that the 3rd order hyperbolic residual-distribution scheme does not require high-order curved grids, which has traditionally been a bottleneck in applying high-order methods for practical problems. These significant advances in methodology are currently being integrated into NASA's FUN3D solver, which is a three-dimensional fully unstructured Navier-Stokes solver. FUN3D is a candidate for inclusion as the near-body solver for HELIOS, the primary DoD/Army rotorcraft CFD analysis code.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. A Mesoscale Dislocation Mechanics Approach to Dynamically Propagating Shear Bands in Metals

Professor Amit Acharya, Carnegie Mellon University, Single Investigator Award

The objective of this research is to develop and demonstrate the fundamentals of a predictive, computational tool for modeling damage due to propagating localized bands of plastic deformation in metals, in particular shear bands, under both high temperature and room temperature conditions. Shear banding in metals has been studied by using well-established elastic and bulk inelastic response functions. However, these responses by themselves along with the conventional theory of elasto-viscoplastic materials are incapable of representing the existence and the propagation of a deformation band tip curve that propagates in the material thereby extending the thin layer of the deformation band. A key goal is to develop an appropriate theory that overcomes this fundamental limitation of conventional theory and its implementation and validation. The objective will be achieved by utilizing a partial differential equation (PDE) based model for plastic deformation developed on the basis of a kinematical faithful representation of the motion of 'dislocations', understood in this context as a specific spatial gradient of elastic distortion. When such gradients are localized along a cylinder whose axis is a space curve, as e.g. at the boundary of a layer of intense plastic deformation where the intensity of the deformation diminishes smoothly over a small distance, the resulting smooth tip of the deformation band is called a (non-singular) dislocation curve. For crystalline materials, the model is rooted in the representation of defects in the crystal lattice at the atomic scale and, through commonly used filtering approaches, provides a pathway to pose space-time averaged PDE models at the meso and macro scales. At every scale, there is an entity/field in the model representing the dislocation density that is a density of curves carrying a vectorial attribute. Moreover, the mechanical structure of the theory and thermodynamic considerations provide a driving force for the velocity of the dislocation density field which, for the situation when a dislocation density field is localized as a non-singular curve (e.g. along a notch tip in a loaded specimen), has the property that it moves the curve perpendicular to itself in space. This has the effect that the deformation band extends exactly along the path of the band-tip (the curve along which the dislocation density is localized), thus producing a propagating band of plastic deformation. As can be clearly seen, conventional elastoplasticity theory simply does not have equations that can produce such behavior that is, however, widely observed in real applications.

In FY16, it is anticipated that the research team will develop an efficient FEM implementation for finite deformation (M)FDM theory. This shall include accounting for finite anisotropic elasticity (that accounts for pressure dependence of second-order elastic moduli), the wealth of classical mechanics of materials knowledge (both constitutive and modeling) related to accounting for rate-dependence and thermal softening of the strength of the material.

B. Managing Uncertainty: Principles for Robust and Dexterous Continuum Mechanics

Professor Annette Hosoi, Massachusetts Institute of Technology, Single Investigator Award
Co-PIs: Professor Russ Tedrake, MIT, and Professor L. Mahadevan, Harvard University

The objective of this research is to explore the underlying scientific principles of programming continuously deformable structures to perform rich and diverse interactions with the physical environment. In particular, researchers will focus on interactions with diverse geometries (as in object manipulation, or locomotion on terrain) with an emphasis on uncertainty: having imperfect knowledge of the geometric, inertial, and impedance properties of the objects or environment, as well as limited, noisy proprioception and actuation. The scientific approach will be guided by biology, taking inspiration from biological counterparts and quantifying the relative performance of our engineered and model systems. Several projects will be ongoing in FY16:

In the first project, the team will conduct an experimental and theoretical study of a new mode of locomotion in snakes observed in juvenile anacondas. This mode is a rapid escape strategy wherein the snake forms an S-shape and, by partly lifting its body, slithers through this shape without ever sliding relative to the ground. While superficially similar to sidewinding, this locomotion mode is qualitatively different because it is a transient mode that allows the snake to move parallel to itself and does so by having just a single point of application rather than in sidewinding where one has two or three support points and requires a sophisticated neuromuscular strategy.

This mode of locomotion is not seen in adults and raises the natural question of why. To understand this, the team will build a mathematical model of snake locomotion that accounts for out-of-plane motion and assess how the Stigmatic-start is only viable for a range of body sizes (relative to muscle strengths). The team predicts very small snakes will flail and very large snakes will not be able to lift themselves off the ground. This study will allow for the consideration of new methods of actuation and movement in hyper-redundant robots.

In the second project, the team will implement a benchtop experiment of a "soft juggling robot." The robot has a single rotary electric motor moving a one-link manipulator with a soft (elastic band) skin. The experiment will be in a planar configuations (using a puck sliding on low-friction table at a 45 degree angle). One of the main virtues of this models, unlike a finite-element approach, is that the team can do least-squares parameter estimation to estimate a few lumped parameters from a few sample trajectories.

C. Experimental and Quantum Mechanics Investigations for the Development of a Liquid-phase Chemical Reaction Mechanism of RDX

Professor Stefan Thynell, The Pennsylvania State University, Single Investigator Award

The objective of this effort is to develop a detailed liquid-phase decomposition mechanism of RDX which includes only elementary reactions. This research aims to identify the remaining species that are formed in liquid-phase reactions, formulate a detailed liquid-phase, elementary reaction model of RDX based on the identified decomposition species and use of QM calculations, and determine the activation energies and pre exponential factors of the assumed reactions using the conventional transition state theory and tunneling corrections, and if computationally feasible, the variational transition state theory. It is anticipated that in FY16 thermolysis data will be acquired by both the FTIR and ToFMS spectrometers. The individual spectral data are to be interpreted, and the series of spectra from a given test are processed into temporal data (species concentration versus time). The information obtained from the experiments will then be used to guide the QM calculations and various levels of theory is used in order to check the results on the identified transition states. Calculations of transition states for both liquid and gas phases will be performed in order to transfer data and improve the RDX gas-phase mechanism.

D. Dynamics of Turbulent Taylor-Couetter Flow via Exact Navier-Stokes Solutions

Professor Roman Grigoriev, Georgia Institute of Technology, Single Investigator Award

The objective of this research is to test the feasibility of a relatively new description of turbulence called Exact Coherent State (ECS). This framework posits that features of classically observed coherent structures can be described using the language of dynamical systems, namely that ECS represent equilibria, traveling waves, and periodic orbits. As such, turbulent dynamics may be able to be understood as a series of transitions between ECS along a network of dynamical connections formed by the intersections of their stable and unstable manifolds. If such a description can be formulated, promise to revolutionize the field of fluid dynamics by providing low-dimensional descriptions of the infinite-dimensional state space that is a turbulent flow.

It is anticipated that in FY16, an adjoint-based generalized minimal residual solver will be developed and integrated into the solver used to compute and analyze Taylor-Couette flows, which are the model flows under investigation. The new numerical methods are necessary in order to couple the best techniques for computing both the flowfields and the ECS. Additionally, the code's boundary condition treatments will be modified in order to provide mechanisms to trigger transitions between computed ECS. This will allow the connections between the ECS to be explored to understand how the flow evolves from one state to the next. Construction of these tools are critical to enable rigorous exploration of whether ECS can provide a practical framework for understanding turbulent flow phenomena.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Ralph Anthenien
Division Chief
Program Manager, Propulsion and Energetics

Dr. Samuel Stanton
Program Manager, Complex Dynamics and Systems

Dr. Asher Rubinstein
Program Manager, Solid Mechanics

Dr. Matthew Munson
Program Manager, Fluid Dynamics

B. Directorate Scientists

Dr. David M. Stepp
Director (Acting), Engineering Sciences Directorate

Dr. April Brown (IPA)
Research Scientist

Mr. George Stavrakakis
Contract Support

C. Administrative Staff

Ms. Pamela Robinson
Administrative Support Assistant

CHAPTER 10: NETWORK SCIENCES DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2015* is to provide information on the programs and basic research supported by ARO in fiscal year 2015 (FY15), and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Network Sciences Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY15.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Network Sciences Division supports research to discover mathematical principles to describe, control, and to reason across the emergent properties of all types of networks (*e.g.*, organic, social, electronic) that abound all around us. The unprecedented growth of the internet, the tremendous increase in the knowledge of Systems Biology, and the availability of video from US military operations have all led to a deluge of data. The goal of the Network Sciences Division is to identify and support research that will help create new mathematical principles and laws that hold true across networks of various kinds, and use them to create algorithms and autonomous systems that can be used to reason across data generated from disparate sources, be they from sensor networks, wireless networks, or adversarial human networks, with the resulting information used for prediction and control. Given that network science is a nascent field of study, the Network Sciences Division also supports basic research on metrics that are required to validate theories, principals and algorithms that are proposed.

2. Potential Applications. Research managed through the Network Sciences Division will provide the scientific foundation to create revolutionary capabilities for the future warfighter. In the long term, the basic research discoveries uncovered by ARO through network science research may provide new and revolutionary tools for situational awareness for the Solider and new regimes for command, control and communication for the Army. Furthermore, work supported by ARO through the Network Sciences Division could lead to autonomous systems that work hand-in-glove with the Soldier.

3. Coordination with Other Divisions and Agencies. To effectively meet the Division's objectives, and to maximize the impact of potential discoveries for the Army and the nation, the Network Sciences Division frequently coordinates and leverages research within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), and the Defense Advanced Research Projects Agency (DARPA). In addition, the Division frequently coordinates with other ARO Divisions to co-fund research, identify multi-disciplinary research topics, and to evaluate the effectiveness of research approaches. For example, interactions with the ARO Computing Sciences Division include promoting research to investigate game-theoretic techniques that could lead to better cyber situational awareness and to address concerns about performance and resilience to cyber attacks in ad-hoc dynamic wireless networks in a uniform fashion. The Network Sciences Division also coordinates its research portfolio with the Mathematics Division to pursue studies of game theory that address bounded rationality and human social characteristics in a fundamental way. The Network Sciences Division coordinates with Life Sciences on studies at the neuronal level to understand human factors in how decisions are made under stress. Lastly, the Division's Program Areas interface with the Mechanical Sciences Division to understand the interplay between learning and manipulation and locomotion in robotic systems. These interactions promote a synergy among ARO Divisions and improve the goals and quality of each Division's research areas.

B. Program Areas

The Network Sciences Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY15, the Division managed research within these four Program Areas: (i) Multi-agent Network Control, (ii) Decision and Neuro Sciences, (iii) Communications and Human Networks, and (iv) Intelligent Networks. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term objectives that collectively support the Division's overall objectives.

1. Multi-agent Network Control. The Multi-Agent Network Control program has a long, successful history in providing new scientific results and leadership concerning the mathematical foundations for the robust control of complex real-time physical and information-based systems. The program was among the first in the DoD to recognize the need and potential for mathematical control theory to be pushed toward the heterogeneous multi-agent and (semi)autonomous domain, leading to a strong record of success in the distributed control of autonomous agents as well as the control of micro-biological systems. Concurrent with these developments, the scientific community became keenly aware of the role of interconnections, and dynamics over these interconnections, on the ensuing behavior of finite (oftentimes large) numbers of agents (in the abstract sense). This subsequently led to the burgeoning discipline of "network science" for which principles were sought and discovered and often found a broad range of applications spanning the physical, biological, and social sciences. While discovery and understanding of complex systems in nature, economics, and society are of profound value and impact, our ability to exploit this knowledge to engineer the controllability, fragility, propensity for self-organization, and/or robustness of interdependent dynamical systems will inevitably demonstrate true mastery. Creating the relevant theory to adapt and control science in this regard has emerged as a focal point for future programmatic efforts. An overarching, principled framework has yet to be established and requires not only control theory, but also dynamical systems, information processing, and phenomenological physics. Thus, the mission of the Multi-Agent Network Control program is to establish the physical, mathematical, and information processing foundations for the control of complex networks. In view of complementary ARO Network Science Division efforts spanning intelligent, communication, and sociological networks, the main focus of the program will primarily involve physical and biological networks but in an abstract framework potentially extensible to network models relevant to all division portfolios. This Program Area is divided into three research thrusts: (i) Control and Dynamical Systems Theory, (ii) Information Structure, Causality, and Dynamics, and (iii) Physics in the Control of Complex Networks. These thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long-term goal.

2. Social and Cognitive Networks. The goal of the Social and Cognitive Networks program is to develop measures, theories, and models that capture cognitive and behavioral processes that lead to emergent phenomena in teams, organizations, and populations. Social networks allow collective actions in which groups of people can communicate, collaborate, organize, mobilize, or attack. Social influence processes determine how ideological groups form and dissolve, information and beliefs spread and interact, and how populations reach consensus or contested states. Research supported in this program includes both methodological aspects of modeling human networks and substantive work to further our understanding social and emergent phenomena. Methodological projects focus on statistical network analysis, computational models and dynamic simulations that address issues such as scalability, multilayers, and data accuracy (i.e., investigating effects of measurement error on metrics and inferences due to missing, inaccurate or hidden network data). Substantive research focuses on cognitive and psychological factors that drive social phenomena, including development of new metrics, constructs and mechanisms involved with complex activities such as information transfer/exchange and collective decision-making. This program invests in innovative solutions that blend theories and methods from the social sciences with rigorous computational methods from computer science and mathematical modeling. The changing nature of DoD's doctrines and missions have greatly increased the need for models that capture the cognitive, organizational and cultural factors that drive activities of groups, teams and populations. The program seeks to advance our understanding of the human dimension and provide critical insights about team coordination and problem solving, social diffusion and propagation, and develop tools that enable inference and modeling of complex social phenomena.

3. Communications and Human Networks. The goal of this Program Area is to better understand the fundamental scientific and mathematical underpinnings of wireless communications and human networking, their similarities, and the interactions between these two networks. This Program Area is divided into two research Thrusts: (i) Wireless Communications Networks and (ii) Human Networks. These Thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research to pursue the program's long-term goal. The Wireless Communications Networks Thrust supports research to discover the fundamental network science principles as they apply to the wireless multi-hop communications systems, while the Human Networks Thrust identifies and supports research to better understand social network structures from heterogeneous data, the structures effect on decision making, and the interaction of communications and human networks. The research efforts promoted by this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications could include wireless tactical communications, improved command decision making, and determining the structure of adversarial human networks.

4. Intelligent Networks. The goal of this Program Area is to develop and investigate realizable (i.e., computable) mathematical theories, with attendant analysis of computational complexity, to capture common human activity exhibiting aspects of human intelligence. These studies may provide the foundation for helping augment human decision makers (both commanders and Soldiers) with enhanced-embedded battlefield intelligence that will provide them with the necessary situational awareness, reconnaissance, and decision making tools to decisively defeat any future adversarial threats. This Program Area is divided into two research Thrusts: (i) Integrated Intelligence and (ii) Adversarial Reasoning. These thrusts guide the identification, evaluation, and monitoring of high-risk, high payoff research efforts to pursue the program's long term goal. The Integrated Intelligence Thrust supports research to discover the mathematical structuring principles that allows integration of the sub-components of intelligent behavior (such as vision, knowledge representation, reasoning, and planning) in a synergistic fashion, while the Adversarial Reasoning Thrust area brings together elements of Game Theory, knowledge representation and social sciences to reason about groups/societies in a robust manner. The research efforts promoted by this Program Area will likely lead to many long-term applications for the Army, the nation, and the world. These applications could include robotic unmanned ground and air vehicles, reasoning tools for wild life management, and decision making tools in the context of command, control, communications, computers, intelligence, surveillance and reconnaissance (C4ISR).

C. Research Investment

The total funds managed by the ARO Network Sciences Division for FY15 were $47.5 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY15 ARO Core (BH57) program funding allotment for this Division was $4.8 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $5.4 million to projects managed by the Division. The Division also managed $31.8 million of Defense Advanced Research Projects Agency (DARPA) programs, $1.7 million of Congressional funds, and $1.5 million was provided by other Army Laboratories. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $0.3 million for contracts. Finally, $2.0 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.2 million of ARO Core (BH57) funds, in addition to any funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY15 (*i.e.*, “new starts”), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY15 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY15, the Division awarded 20 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Francois Baccelli, University of Texas at Austin; *The Laws of Opinion Dynamics in Social Systems: Theory and Inference*
- Professor Noshir Contractor, Northwestern University; *Socio-Cognitive Networks: Theory & Data Driven Approaches for Understanding the Assembly and Interaction Networks of High Performance Teams*
- Professor Massimo Franceschetti, University of California - San Diego; *Human Networks: From Algorithmic Models to Global Behavior*
- Professor Aram Galstyan, University of Southern California; *Networks as Encodings of Social Attributes: Inference and Fundamental Limits*
- Professor Wei Gao, University of Tennessee at Knoxville; *Adaptive Mobile Networking at the Tactical Edge: A Social-Aware Perspective*
- Professor Georgios Giannakis, University of Minnesota - Minneapolis; *Comprehensive Tactical Network State Inference from Incomplete Data*
- Professor Eric Gilbert, Georgia Tech; *Modeling and Detecting Online Rumors*
- Professor Paolo Grigolini, University of North Texas; *Behavioral Constraints on Game Theory*
- Professor Mohammed Hoque, University of Rochester; *Automated Modeling of Deceptive Intent in Computer-Mediated Conversations*
- Professor I-Hong Hou, Texas A&M; *Towards Provably Timely and Reliable Networks*
- Professor Negar Kiyavash, University of Illinois - Urbana-Champaign; *Casual Inference in Complex Networks*
- Professor Kristina Lerman, University of Southern California; *Quantifying Cognitive Factors in Online Social Behavior*
- Professor Adilson Motter, Northwestern University; *Properties Controlling Synchronization in Networks of Dynamical Systems*
- Professor Michael Pursley, Clemson University; *Efficient Delivery of Information in Networks*

- Professor Artemio Ramirez, University of South Florida; *The Nature of Relationship Reconnection in Social Networks: Documenting the Process of Reactivating Dormant Ties*
- Professor Lev Reyzin, University of Illinois - Chicago; *Learning and Inferring Networks from Incomplete Data*
- Professor Paulo Shakarian, Arizona State University; *Understanding Social Influence without Markov Assumptions*
- Professor Gabriel Silva, University of California - San Diego; *Inference and Control of Network Dynamics from Network Structure and Geometry*
- Professor Milind Tambe, University of Southern California; *Building a Science of Cyber-Security Games*
- Professor Ufuk Topcu, University of Texas at Austin; *Probably Approximately Correct Protocols for Reactive Control and Learning*

2. Short Term Innovative Research (STIR) Program. In FY15, the Division awarded three new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Francesco Bullo, University of California - Santa Barbara; *Dynamic Processes over Dynamic Social Networks*
- Professor Sanjay Shakkottai, University of Texas at Austin; *Large-scale Social Network Analytics with Limited Expert Input*
- Professor Nikolaos Sidiropoulos, University of Minnesota - Minneapolis; *Factor Analysis for Spectral Reconnaissance and Situational Understanding*

3. Young Investigator Program (YIP). In FY15, the Division awarded three new YIP projects to drive fundamental research in areas relevant to the current and future Army. The following PIs and corresponding organizations were recipients of the new-start YIP award/awards.

- Professor Daniel Lowd, University of Oregon; *Inferring Trustworthiness and Deceit with Adversarial Relational Models*
- Professor Konstantinos Pelechrinis, University of Pittsburgh; *Models and Metrics for Composite Socio-Spatial Networks*
- Professor Emma Spiro, University of Washington; *Mass Convergence of Attention During Crisis Events: Degree Dynamics and Emergency Response in Online Settings*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY15 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *NetSci-X 2015*; Rio de Janeiro, Brazil; 14-16 January 2015
- *6th Workshop on Complex Networks (CompleNet 2015)*; New York, NY; 25-27 March 2015
- *Sampling Theory and Applications (SampTA 2015)*; Washington, DC; 25-29 May 2015

5. Special Programs. In FY15, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded four new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These awards constitute a significant portion of the basic research programs managed by the Network Sciences Division; therefore, all of the Division's active MURIs are described in this section.

1. Neuro-Inspired Adaptive Perception and Control. This MURI began in FY10 and was awarded to a team led by Professor Panagiotis Tsiotras of the Georgia Institute of Technology, with participation from researchers at the Massachusetts Institute of Technology and the University of Southern California. The objective of this MURI is to investigate a new paradigm based on “perception/sensing-for-control” to achieve a quantum leap in the agility and speed maneuverability of vehicles. The team will leverage attention-focused, adaptive perception algorithms that operate on actionable data in a timely manner; use attention as a mediator to develop attention-driven action strategies (including learning where to look from expert drivers); analyze the saliency characteristics of a scene to locate the important “hot-spots” that will serve as anchors for events; make use of fused exteroceptive and proprioceptive sensing to deduce the terrain properties and friction characteristics to be used in conjunction with predictive/proactive control strategies; and will study and mimic the visual search patterns and specialized driving techniques of expert human drivers in order to develop perception and control algorithms that will remedy the computational bottleneck that plagues the current state of the art.

This MURI will have significant benefits for the Army in the field and off the field, such as increasing vehicle speed and agility in direct battlefield engagements, as it will increase the chances of evading detection by the enemy or of escaping an ambush. As confirmed by several Army studies, the difficulty of successfully engaging and hitting a target increases disproportionately with the target speed. Support logistics will also become safer and more effective as even moderate increases in speed can largely increase the capacity of convoys and the throughput of the supply lines of materiel. Finally, the results of this research will contribute to the development of realistic off-road high-speed simulators for training special forces and other military and government personnel.

2. Scalable, Stochastic and Spatiotemporal Game Theory for Adversarial Behavior. This MURI began in FY11 and was awarded to a team led by Professor Milind Tambe of the University of Southern California, with participation from researchers at UCLA, Duke University, Stanford University, UC Irvine and California State University at Northridge. The objective of this MURI is the development of game theory formalisms that account for bounded rationality, scalability of solutions, real-world adversaries, and socio-temporal issues. The technical approach to be followed by the team will involve a mix of behavioral experiments and development of theoretical formalisms to characterize individual human behavior and that of adversarial groups; it is expected that psychological theories such as prospect theory and stochastic theories for coalitional games will play equal part in the technical development. The results of this MURI may have significant impact on diverse applications of the Army such as the monitoring of contracts while building nations or societies.

3. Evolution of Cultural Norms and Dynamics of Socio-Political Change. This MURI began in FY12 and was awarded to a team led by Professor Ali Jadbabaie of the University of Pennsylvania, with participation from researchers at MIT, Stanford, Cornell, and Georgia Tech. The objective of this MURI is to find synergy in methods and models from work in social sciences, engineering, network sciences, and mathematics to develop new techniques and mathematical models that would explain societal events not *posterior* but as they are happening, based on detailed analytical models of social systems. The team hopes to use a unified yet interdisciplinary lens that goes beyond social and political sciences, and adequately covers the full spectrum from rigorous math-based theory and modeling to large scale data extraction and analyses and from multi-agent simulation to controlled lab experiments and field surveys. The results of the MURI may have significant impact on the Army and DoD to understand cataclysmic changes, such as the Arab Spring, as they are about to happen.

4. Control of Complex Networks. This MURI began in FY13 and was awarded to a team led by Professor Raissa D’Souza of the University of California at Davis. The goal of this MURI project is to develop rigorous principles to predict and control behaviors of systems made of interdependent networks. This will be accomplished through an interdisciplinary approach synthesizing mathematical theories from statistical physics, control theory, nonlinear dynamics, game theory, information theory, system reliability theory, and operations research. The results will be informed and validated by empirical studies of real-world systems from nanoscale mechanical oscillators, to collections of interdependent critical infrastructure systems, to data on coalitions and conflict in primate societies, to longitudinal data on the evolution of political networks of nation states and task-oriented social networks in open source software. The focus is to develop new approaches that exploit network interdependence for network control, and this diversity of empirical testbeds is central to developing robust theoretical principles and widely applicable methods.

It is expected that this MURI will lead to (i) network interventions that prevent cascades of failure in critical infrastructures, (ii) novel control schemes relying on control actions and local interventions, (iii) rigorous principles for multi-modal recovery of heterogeneous systems, (iv) shaping human social response via designed incentives that align human behavior with the capabilities of technological networks, (v) design of networks of nonlinear nanoelectromechanical oscillators that exploit coupling and nonlinearity to create coherent motion, (vi) new mathematical structures for representing and analyzing networks-of-networks, especially with respect to control theory, and (vii) fundamental bounds on controllability of interdependent networks and rigorous techniques to identify which network layers are easiest to steer.

The anticipated impact on DoD Capabilities is broadly applicable to controlling a disparate collection of autonomous agents interacting through numerous networks in noisy, dynamic environments with a myriad of time-scales and length-scales. Results can be applied to security (and restoration) of critical infrastructures, supply chains, political alliance dynamics (including upheavals such as Arab Spring), conflict, risk, social dynamics, and collective action. It is also reasonable to expect that there will be new levels of nanoscale functionality in the NEMs device developed, enabling new technologies and devices.

C. Small Business Innovation Research (SBIR) – New Starts

Research within the SBIR program have a more applied focus relative to efforts within other programs managed by ARO, as is detailed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY15, the Division managed two new-start SBIR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of two Phase I contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY15 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY15, the Division managed two new-start STTR contracts, in addition to active projects continuing from prior years. The new-start projects consisted of two Phase I contracts. These new-start contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY15 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY15, the Division managed three new ARO (Core) HBCU/MI projects, and four new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The PECASE winners for each year are typically announced by the White House at the end of the calendar year. However, the FY13-FY15 PECASE recipients had not yet been announced by the end of FY15. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY15, the Division managed four new DURIP projects, totaling $0.6 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. DARPA Anomaly Detection at Multiple Scales (ADAMS) Program

The ADAMS program is an effort to understand how insider threats to an organization (such as Nadal Hassan or Robert Hansen) can be predicted based on changes in behavior of individuals, or a small group of people within an organization. At a technical level this program involves mining incredibly large graphs (based on normal human activity) in a manner that is cognizant of human behavior, which reduces to computational challenges in managing and reasoning of large datasets, statistical reasoning techniques to find black swans, and efforts to manage uncertainty in both data and reasoning techniques. This program is managed on behalf of DARPA through the Network Sciences Division, Intelligent Networks Program.

I. DARPA Structured Social Interactions Module (SSIM) Program

The SSIM program is an effort to discover what makes certain soldiers, policemen and ethnographers effective in new environments (*e.g.*, a different culture to their own) making them "Good Strangers." Typically, Good Strangers can operate in a new environment without upsetting the local population and are good at understanding social mores without being taught what they are. This program engages social scientists to identify physiological coping mechanisms and psychological characteristics of Good Strangers, and artificial intelligence experts to devise new Social Science cognizant computer-based simulation and training algorithms. This program is managed on behalf of DARPA through the Network Sciences Division, Intelligent Networks Program.

J. DARPA Social Media in Strategic Communication (SMISC) Program

The SMISC program is an effort to understand and control strategic communication that takes place over social media. Recent events in Madagascar, North Africa (especially the Arab Spring) and in Bangalore suggest that social media could and does play a major role in bringing together mobs and crowds in unpredictable ways. The SMISC program aims to develop solutions that could be used to understand development of memes over social media and potential techniques to influence the formation or dissipation of memes. This program is managed on behalf of DARPA through the Network Sciences Division, Intelligent Networks Program.

K. DARPA Big Mechanism Program

The Big Mechanism program attempts to understand conflicting information available in research literature on any big mechanism. The chosen area for the program is Cancer Biology, while the resulting techniques could be applied to a number of other mechanisms including climate change, with each piece of published work contributing a small portion of understanding to the big mechanism. The effort should lead to advances in the Natural Language Processing for automatically extracting information for scientific literature, advances in knowledge representation for signaling pathways with potential ambiguities in cancer biology, resolution of information from new publication against what is already known, and potential for advancement in explanation of causality of how cancer cells grow. This program is managed on behalf of DARPA through the Network Science Division, Intelligent Networks Program.

L. DARPA SIGMA Program

The SIGMA program is an effort to understand the issues associated with deploying a large sensor network for detection of nuclear threats in an urban environment. The concept of the program is to develop a very large network of sensors, that can be carried by people, but require no interaction. The program includes development of the sensors, communication networking via smart phone devices, and processing and fusing very large amounts of data. Communications and networking issues include security and privacy as well as dealing with data transfer from a large number of sensors. Portions of this program dealing with the sensor communications and networking as well as research into human factors dealing with technology adoption are managed on behalf of DARPA through the Network Sciences Division, Communications and Human Networks Program.

M. DARPA Communicating with Computers (CwC) Program

The goals of the DARPA Communicating with Computers program are to advance the state of the art in text and video analytics to the extent that a machine and its human operator can have the same mental model. This requires that the machine be able to understand the human intent, and that it can explain back, to the human, in ways that makes use of the context and prior knowledge. Three challenge problems have been chosen: (i) playing a game of blocks between humans and machines, (ii) a bicuration assistant that helps a human investigate knowledge representation of signaling pathways in cancer biology, and (iii) an author's assistant that could help a human write stories. This program is managed on behalf of DARPA through the Network Science Division, Intelligent Networks Program.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Network Sciences Division.

A. Millimeter Wave Mobile Ad Hoc Networks

Professor Robert Heath, University of Texas - Austin, Single Investigator Award

Millimeter wave (mmWave) communication will use high-bandwidth and directional antenna arrays to achieve large data rates. While the theoretical bit rate is incredible, which can allow the sharing of high-resolution video in a tactical military network or file sharing in a peer-to-peer network, several engineering hurdles remain. In previous generations, interference of nearby users limited performance of ad hoc networks. The properties of mmWave communication, however, offer opportunities to exploit the reduced interference created by directional antennas and building blockage. The goal of this research is to understand the true capacity of a mmWave network in a tactical environment. From this capacity, the benefits of pursuing the development of mmWave communications for military specific applications can be determined.

In FY15, Professor Heath derived a Signal to Interference and Noise Ratio (SINR) complimentary cumulative distribution function (CCDF) in order to derive the transmission capacity in an outdoor environment, with directivity and blockages. The ergodic capacity of an outdoor mmWave ad hoc network was quantified from the resulting bound on the CDF of the SINR. Using tools from stochastic geometry, an expression is derived for the ergodic capacity that matches simulation results for both line-of-sight (LOS) and non-line-of-sight (NLOS) communication. The inevitable problem of beam misalignment was formally modeled in mmWave ad hoc networks, resulting in a simple expression that captures the loss of capacity for small alignment error. The impact misalignment errors on the ergodic capacity of the network have been quantified and compared with standard sectored antenna models.

B. Social Network Processes in Collaborative Decision Making

Professor Chris Riedl, Northeastern University, Young Investigator Award

The objective of this research is to determine optimal organizational configurations for humans engaged in complex problem solving tasks. In FY15, Professor Chris Riedl at Northeastern University used agent-based modeling to answer fundamental questions about how best to organize people to solve difficult problems. Virtual experiments were run with 100 agents placed on a relatively smooth NK fitness landscape (N=20, K=5) and varied with respect to (a) network typology, (b) risk taking search strategy, and (c) heterogeneity of risk taking strategies. Results from this research revealed that risk taking behavior with respect to landscape exploration is beneficial to performance (see FIGURE 1). Further, the results of this research suggest that strongly connected communication networks can lead to rapid convergence on local maxima, while weakly connected networks perform poorly at first and outperform strongly connected networks over longer time spans. However, results show that when the population of agents are homogeneous in risk taking behavior and they take moderate risks (increasing their one-step exploration range from 1 unit to 2-5 units), strongly connected networks outperform weakly connected networks, likely due to the increased ability of an agent to “jump” out of a local optima solution, while also having a strong network of support if that jump is unsuccessful.

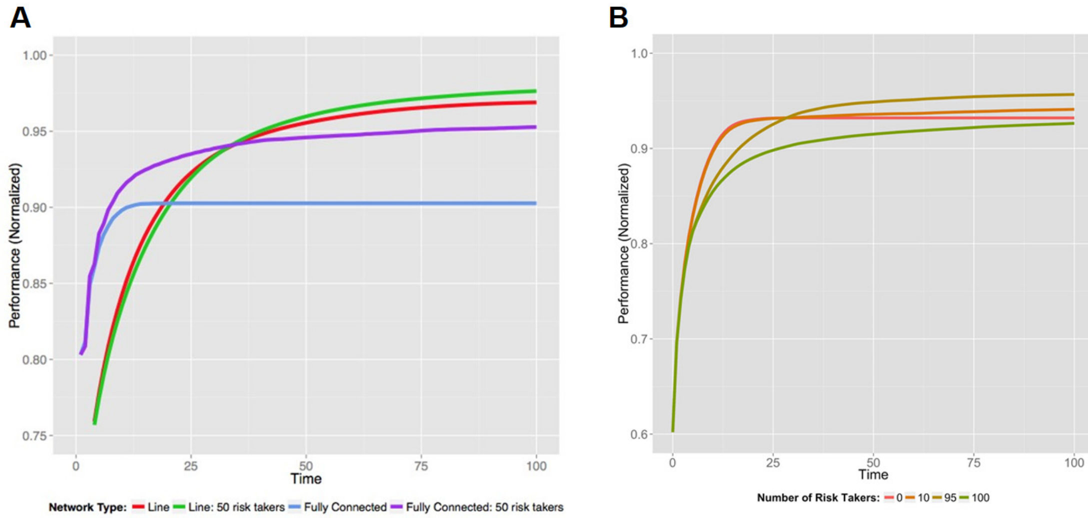

FIGURE 1

Risk taking behavior with respect to landscape exploration is beneficial to performance. (**A**) The effects of risk takers is plotted based on network type. The difference in performance between the linear and fully connected network with no risk takers is quite large (approx. 0.07 at Time 100), and drops to 0.025 when 50 risk takers are added to each network. (**B**) In a small world network with k = 2, 50 rewires, simulations with 100 risk takers perform worst, followed by simulations with 0 risk takers. The heterogeneous runs with 10 and 95 risk takers perform best.

The presence of heterogeneity in agent risk taking behavior leads to better results than any of the homogeneous cases. Further, the exact distribution of risk heterogeneity may not be of foremost importance; simply having some variability, low and medium risk takers in the network is enough for near optimal performance. This research makes important contributions to the literature on collaborative work and collective decision making by investigating the impact of agents' search strategy in decision making situations that suffer from uncertainty. This research also contributes to a better understanding of the changing nature of work in which large groups of agents operate as self-organized systems.

C. Ergodic Control for Optimal Information Acquisition

Professor Todd Murphey, Northwestern University, Single Investigator Award

The objective of this research is to develop an active search process that incorporates information measures into trajectory design to estimate the state of continuous, time-varying fields. Nonlinear optimal control theory plays a central role, and the goal of the research is to develop the tools necessary to select continuous-time trajectories for systems with nontrivial dynamics - for instance, systems with nonholonomic constraints or significant inertial effects. The developed techniques use measures of ergodicity and the associated ergodic control to robustly explore for information while ensuring coverage of the informative subset of the state space (as indicated by prior measurements or even the lack thereof). The methods developed will provide a synthesis technique for active sensing so that autonomous systems can optimize knowledge of continuous phenomena such as fluid or air flow fields, chemical dispersion, magnetic fields, electric fields, and other continuum phenomena. Further, by developing trajectories that enable fast and accurate estimation of the state and evolution of such fields in local regions, the research can support forecasting and prediction. This goal was split into several sub-goals: (i) how can infinite dimensional fields be represented and explored?; (ii) when fields and/or parameters are time-varying, how does ergodic planning change?; (iii) when fields and/or parameters are time-varying, how does the expected information density evolve with time?; (iv) how can the use of Fourier techniques in the spatial domain be reduced or eliminated?; and (v) why is information maximization not as robust as ergodic exploration?

In FY15, significant progress was made on sub-goals (i), (ii), and (iii). Researchers learned that ergodic control is effective in handling dynamic constraints of various types, demonstrated ergodic control using traditional sensing models such as range sensing, and developed a version of ergodic control for time-varying distributions. The first important result is that ergodic control is as effective for nonlinear systems as it is for linear systems (see FIGURE 2). For instance, the computation of ergodic control in the context of a weakly electric field sensor for a fully-actuated linear system leads to very different trajectories than that of a simple nonholonomic vehicle model. Nevertheless, the information evolution ends up being nearly identical.

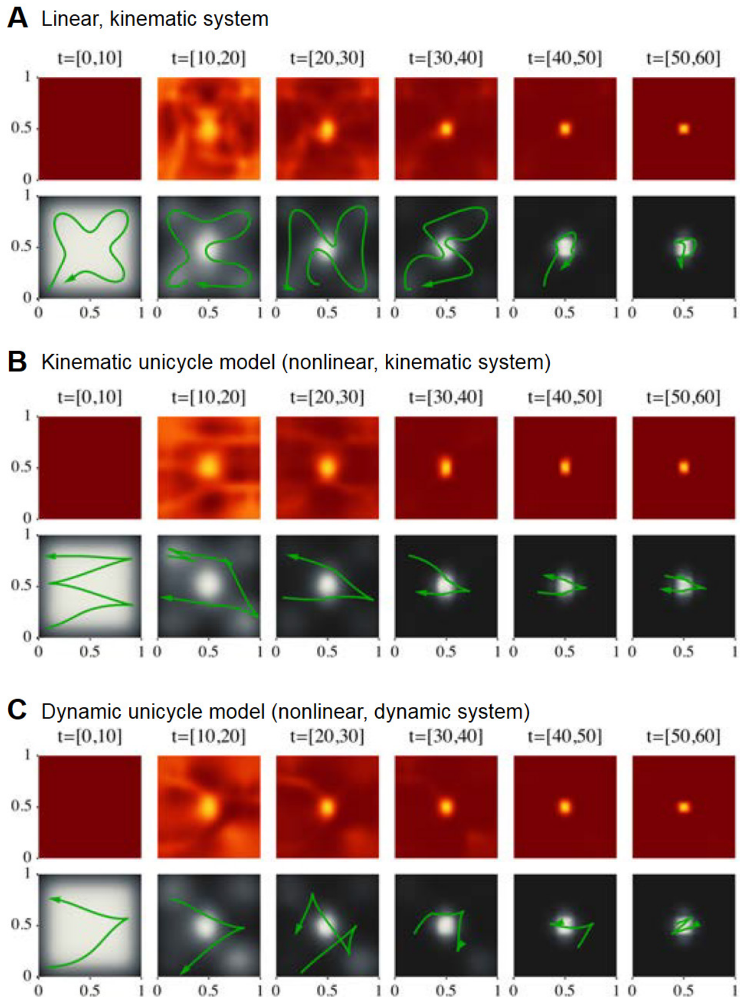

FIGURE 2

Advances in ergodic control: A progression of the estimate of the two-dimensional target location using the newly developed ergodic exploration of distributed information algorithm, in simulation, for three different systems performing the same task. As the algorithm progresses, collected measurements evolve the estimate (heatmap) from a uniform distribution over the workspace (top left most figure in each (**A**),(**B**),(**C**)), to a concentrated distribution at the correct location. At each interval, the expected information density (grayscale) is calculated from the updated estimate, which is then used to calculate an ergodic search trajectory (green).

An important question was whether ergodic exploration has any advantage for more standard sensor types (e.g., range sensing). The measurement models for these sensors are comparably linear, so it was possible that ergodic control would only have practical benefit for exotic sensors like weakly electric field sensing. However, ergodic sensing leads to substantial robustness, particularly with respect to distractions in the environment. One of the main areas that was considered is what happens when a field is time-varying. Professor Murphey investigated the problem of a group of agents, or equivalently a set of particles representing the uncertainty with respect to a single agent, and computed ergodic control assuming a model for agent behavior. The agents were able to swarm over a non-convex region. Ergodic control was synthesized using Fourier transforms across the spatial domain as well as the time domain. Interestingly, this approach easily led to an effective control strategy, without modifying any of the original optimal control analysis developed for stationary information maps. Of the mathematical results, the most important is that the ergodic metric has been shown to be convex, and that it is convex even if only a finite set of Fourier basis functions are used. This is one step towards showing that ergodic control can be expected to be well posed in general.

D. Semantic Characterizations of Failures and Beliefs of Machine Perception Systems

Professor Devi Parikh, Virginia Tech, Young Investigator Program

Autonomous systems that depend upon machine learning, unfortunately, fail miserably when encountering new situations that they have not been trained on. Autonomous systems are made of multiple components – vision, planning, mobility, and dexterity – that work collaboratively. Failure in one component, typically, propagates to other components leading to catastrophic failure of the entire system. While there have been efforts to improve machine learning in each component, using techniques such as domain adaptation, failures do not allow an orderly shutdown. An alternative, explored by Prof. Parikh, is for a component to provide an explanation of its decision (including aspects of input parameters, and confidence level in its decision) so that other components can use that information to ignore, modify, or ask for new processing. This is especially true of vision systems in robots, whose output is used by a host of other subsystems. In order to rectify catastrophic failures, and to degrade gracefully, autonomous systems need to be endowed with the ability to reflect upon their internal status.

In FY15, Prof. Parikh developed an alert system for every vision algorithm, which can be used to predict its failure. The alert system, constructed as a machine learning algorithm, can be used in tandem with the original vision algorithm to improve robustness of autonomous systems and robots by reducing catastrophic failures by at least 20%. The alert system is based on an analysis of the input to the vision system rather than a post-hoc analysis of the output. By adopting such an approach, the alert system can be constructed for all vision systems, whether they are based on machine learning or not. The results of this research are being incorporated into vision algorithms of the Robotics CTA.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Event Detection in Temporal Social Graphs

Investigator: Professor Leman Akoglu, SUNY Stony Brook, Single Investigator Award
Recipient: Northrop Grumman Aerospace Systems

Ensemble techniques for classification and clustering have long proven effective, yet anomaly ensembles have been barely studied. This research aims to create a new ensemble approach for anomaly mining, with application to event detection in temporal graphs. Professor Akoglu has discovered an ensemble approach for anomaly mining that employs novel techniques to automatically and systematically select the results to assemble in a fully unsupervised fashion. She has successfully used this approach to detect events in temporal graphs derived from social media data, such as Twitter and email feeds. Northrup Grumman Aerospace Systems (NGAS) has developed the code to implement the detection algorithm and has worked with Professor Akoglu to test it using NGAS simulated sensor data. NGAS plans on further developing this tool and build on on-line interface.

B. New Laws of Explosive Networks and Opinion Dynamics

Investigator: Professor Raissa D'Souza, University of California at Davis, MURI Award
Recipient: ARL Computing and Information Sciences Directorate (ARL-CISD)

The objective of this research is to develop a new theory for the sudden emergence of connectivity in complex networks that could lead to new methods for control. Scientists in the Army Research Laboratory's Network Sciences Division worked with the sponsored researchers to extend the theory to social settings, discovering how multiple opinions vying for dominance could lead to counter-intuitive sources of societal instability. Network connectivity is traditionally presumed to happen in a slow, continuous manner. However, the research team discovered that in special cases connectivity might emerge with a bang, not a whimper, via a phenomenon they have dubbed "explosive percolation." While high connectivity in operating systems like the internet or the stock exchange is desirable, in cases such as epidemic spreading or deleterious zealotry, the extent of connectivity needs to be curtailed. Even when high connectivity is desirable it can sometimes backfire, causing a potentially catastrophic collapse of the system. The new theory of explosive percolation provides new understanding for manipulating the onset of long-range connectivity in complex networks through a series of small-scale interactions with dramatic consequences. Collaborations with ARL-CISD have also led to a technical publication on zealotry over social networks.

C. Failure Detection in Vision Systems

Investigator: Professor Devi Parikh, Virginia Tech, Young Investigator Award
Recipient: ARL Robotics Collaborative Technology Alliance (CTA)

The objective of this research is to devise methods for understanding when vision algorithms, which are part of an integrated intelligent system, could fail leading to propagation of errors through the system. If the failure can be predicted than other parts of the system could take appropriate actions so that an autonomous system can fail gracefully. The author carried out the technical work as part of a Young Investigator Program award, and has been invited to participate in ARL's Robotics CTA. She has begun work to transition the technology to the consortium and the alliance, though collaboration with ARL CISD researchers.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Adaptive Mobile Networking at the Tactical Edge

Professor Wei Gao, University of Tennessee, Single Investigator Award

The objective of this research is to investigate and exploit the close coupling between mobile communication networks and human social networks at the tactical edge by leveraging the recent research in multi-genre networks. This analysis interprets warfighters' situational response to the heterogeneous battlefield contexts as their social dynamics, which are defined as the temporal and spatial variations of social relationships among warfighters, and are autonomously characterized from warfighters' contact patterns without manual inputs or configurations.

However, due to the Disconnected, Intermittent, and Limited (DIL) network environment at the tactical edge which makes it hard to maintain persistent end-to-end wireless network connectivity among warfighters, there are many challenges of investigating, formulating, and exploiting such social dynamics for adaptive mobile networking, including: (i) the dynamics of warfighters' contact patterns need to be analytically and accurately formulated; (ii) a unified framework integrating models from multi-genre networks is needed to better characterize social dynamics among warfighters; and (iii) the global coordination and timely information exchange among warfighters is challenging due to the lack of end-to-end network connectivity, but are necessary for adaptive network decisions.

It is anticipated that in FY16, this research will address these challenges through stochastic modeling of various essential characteristics of warfighters' behavior patterns, leading to timely and precise prediction of warfighters' communication needs in the future and designs of adaptive mobile networking strategies at the tactical edge. There are three major research thrusts of this research: (i) Adaptive Contact Prediction: improving the accuracy of contact prediction through formulation of the heterogeneous transient characteristics of warfighters' contact patterns in both temporal and spatial dimensions; (ii) Characterization of Social Dynamics: characterizing the social dynamics among warfighters by exploring the correspondence of various sociological concepts in DIL network environments; and (iii) Adaptive Networking Framework: developing social-aware data dissemination and cooperative caching schemes which autonomously adapt to the social dynamics among warfighters. The network models, protocols, and architecture designs will be evaluated using a hybrid method of tactical trace-based simulations and realistic mobile testbed experimentation.

B. Scalable Temporal Network Models with Population Dynamics: Estimation, Simulation, and Prediction

Professor Zack Almquist, University of Minnesota - Minneapolis, Young Investigator Award

Professor Zack Almquist is developing statistical models to predict population (vertex) and link dynamics in social networks. In FY16, he intends to extend the family of Exponential Random Graph Models (ERGMs) used to model dynamic social network processes by developing theory and software for performing dynamic network analysis, prediction, and simulation. In particular, he will develop a vertex dynamics model to account for population dynamics (nodes entering and exiting the network over time) and their effects on network structure and network outcomes. Lastly, he will explore ways to combine the vertex model with the Temporal Exponential Random Graph Models (TERGMs) to simultaneously account for dynamic populations and dynamic network structures as they evolve over time.

Professor Almquist will test and verify his models with empirical data related to organizational collaboration networks, disaster response networks, and interpersonal communication networks. He intends to use as a test case for a joint vertex and link dynamic model data from a natural disaster to demonstrate the predictability of such a model with respect to the inherently dynamic nature of response teams, local and national organizations and their engagement with each other throughout the duration of the crisis event. This innovative work builds off the highly successful ERGM models to add elements that will better handle missing data and temporal dynamics. Prof. Almquist intends to make his developed models accessible to the scientific community by publishing them as R toolkits (open source statistical software).

C. Co-evolutionary Complex Networks: Dynamical Foundations, Influence, and Control
Professor Joshua Weitz, Georgia Institute of Technology, Single Investigator Award

The concept of network-centric operations plays an essential role in the vision of future military capabilities, raising questions of the role of autonomous systems operating under networked architectures for sensing and computation. Both social and biological networks constitute frameworks for investigation, linking theory and applications. This research focuses on the development of theoretical methods, modeling approaches, and computational algorithms for investigating coevolutionary network dynamics, influence, and control, and is organized around a linked set of research thrusts.

It is anticipated that in FY16, researchers will progress in three areas. First, researchers will investigate the dynamical foundations of coevolution, i.e., in which an evolving network topology reacts in feedback with dynamic processes over the network nodes. In the absence of weak coupling or distinct time-scales, it becomes essential to understand the interaction between these two processes, rather than their behaviors in isolation. Second, Professor Weitz will consider how network influence and control functions affect dynamic network behavior in the face of restricted network resources and limited knowledge about network characteristics. Such influence and control may be mediated by exogenous or endogenous means, e.g., through a collection of collaborating internal nodes. Finally, he will focus on a series of linked applications including virus microbe dynamics and the spread of infectious disease in human populations.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Purush Iyer
Division Chief
Program Manager, Intelligent Networks

Dr. Kathryn Coronges
Program Manager (Acting; Outgoing), Social and Cognitive Networks

Dr. Edward Palazzolo
Program Manager (Incoming), Social and Cognitive Networks

Dr. Samuel Stanton
Program Manager (Acting), Multi-Agent Network Control

Dr. Robert Ulman
Program Manager, Communication and Human Networks

B. Directorate Scientists

Dr. Randy Zachery
Director, Information Sciences Directorate

Dr. Bruce West
Senior Scientist, Information Sciences Directorate

Ms. Anna Mandulak
Contract Support

C. Administrative Staff

Ms. Debra Brown
Directorate Secretary

Ms. Diana Pescod
Administrative Support Assistant

CHAPTER 11: PHYSICS DIVISION

I. OVERVIEW

As described in *CHAPTER 1: ARO MISSION AND INVESTMENT STRATEGY*, the purpose of the Army Research Laboratory (ARL) - Army Research Office (ARO) publication *ARO in Review 2015* is to provide information on the programs and basic research supported by ARO in FY15, and ARO's long-term vision for transitioning basic science research to enable new materials, devices, processes and capabilities for the current and future Soldier. This chapter focuses on the ARO Physics Division and provides an overview of the scientific objectives, research programs, funding, accomplishments, and basic-to-applied research transitions facilitated by this Division in FY15.

A. Scientific Objectives

1. Fundamental Research Goals. The ARO Physics Division supports research to discover exotic quantum and extreme optical physics. The Division promotes basic research that explores frontiers where new regimes of physics promise unique function. Examples such as ultracold molecules, complex oxide heterostructures, attosecond light pulses, and quantum entanglement all represent areas where the scientific community's knowledge must be expanded to enable an understanding of the governing phenomena. The results of this research will stimulate future studies and help to keep the U.S. at the forefront of research in physics.

2. Potential Applications. Research managed by the Physics Division will provide a scientific foundation upon which revolutionary future warfighter capabilities can be developed. The Division's research is focused on studies at energy levels suitable for the dismounted Soldier: the electron Volt and milli-electron Volt range. In the long term, the discoveries are anticipated to impact warfighter capabilities in the area of Command, Control, Communications, Computers, Intelligence, Surveillance, and Reconnaissance (C4ISR). Research advances in the Division can be readily visualized to impact sensor capabilities for increased battlespace awareness and Soldier protection, enhanced navigation, ultra-lightweight optical elements and energy-efficient electronics for decreased Soldier load, increased Soldier awareness, and advanced computational capabilities for resource optimization and maximal logistical support.

3. Coordination with Other Divisions and Agencies. To meet the Division's scientific objectives and maximize the impact of discoveries, the Physics Division coordinates and leverages research within its Program Areas with Army scientists and engineers, the Office of Naval Research (ONR), the Air Force Office of Scientific Research (AFOSR), and the Defense Advanced Research Projects Agency (DARPA). In addition, the Division frequently coordinates with other ARO Divisions to co-fund awards, identify multidisciplinary research topics, and evaluate the effectiveness of research approaches. For example, research co-funded with the Mathematical Sciences Division seeks coherent-feedback quantum control of collective hyperfine spin dynamics in cold atoms. Collaborative research with the Electronics Division is also underway with a goal of understanding high frequency responsiveness of magnetic materials and the engineering of agile radio frequency device concepts. The Physics Division coordinates its research portfolio with AFOSR and DARPA in pursuit of forefront research involving ultracold molecules and optical lattices. The Division also coordinates certain projects with Intelligence Advanced Research Projects Activity (IARPA) and other government agencies. These interactions promote a synergy among ARO Divisions and DoD agencies, and impact the goals and improve the quality of the Division's research areas.

B. Program Areas

The Physics Division drives the creation of new research areas, as well as identifies, evaluates, funds, and monitors research in a range of sub-disciplines. The Division has identified several sub-disciplines, also called

Program Areas, which provide a framework for the evaluation and monitoring of research projects. In FY15, the Division managed research within these four Program Areas: (i) Atomic and Molecular Physics, (ii) Condensed Matter Physics, (iii) Optical Physics and Fields, and (iv) Quantum Information Science. As described in this section and the Division's Broad Agency Announcement (BAA), these Program Areas have their own long-term aspirations that collectively support the Division's overall objectives.

1. Atomic and Molecular Physics. The goal of this Program Area is to study the quantum properties of atoms and molecules and advance a fundamental understanding of exotic quantum behavior. When a gas of atoms is sufficiently cooled, the quantum nature dominates and the atoms behave wave-like rather than a cloud of distinct particles. Accordingly, experiments that were once the sole purview of optics are now possible with matter: interference, lasing, diffraction and up/down-conversion, to name a few. This Program Area explores these concepts with an eye toward enabling new opportunities, such as novel quantum chemistry and atomic devices that exploit quantum behavior. The specific research Thrusts within this Program Area are: (i) State-dependent Quantum Chemistry, (ii) Atomtronics, and (iii) Non-equilibrium Many-body Dynamics. Ultracold gases can be trapped in one, two or three dimensional standing optical waves enabling the exploration of novel physics, quantum phase transitions, and mechanisms operative in condensed matter. In optical lattices, one can also create a new "electronics", called atomtronics, based on atoms and molecules having statistics, mass, charge, and many additional handles not available in conventional electronics. The State-dependent Quantum Chemistry Thrust is not focused on synthesis but rather on the underlying *mechanisms*, such as electronic transport, magnetic response, coherence properties (or their use in molecule formation/selection), and/or linear and nonlinear optical properties. While the notion of taking objects held at sub-Kelvin temperatures onto a battlefield may seem irrational, dilute atomic gases can be cooled to nano-Kelvin temperatures without cryogens like liquid nitrogen or liquid helium. The cooling is accomplished with magnetic traps and lasers. The long-term applications of this research are broad and include ultra-sensitive detectors, time and frequency standards, novel sources, atom lasers and atom holography, along with breakthroughs in understanding strongly-correlated materials and the ability to design them from first principles.

2. Condensed Matter Physics. The objective of this Program Area is to discover and characterize novel quantum phases of matter at oxide-oxide interfaces and at the surfaces and interfaces of topological insulators. Recent studies have shown that interfaces can support quantum phases that are foreign to the bulk constituents. Furthermore the bond angles and bond lengths in complex oxides are controllable at interfaces. In general the interface provides a mechanism for potentially controlling lattice, orbital, spin and charge structure in ways that are not possible in bulk, single phase materials. If these degrees of freedom can be engineered in ways analogous to charge engineering in semiconductors, it will present new opportunities for the development of advanced technologies utilizing states beyond just charge. Topological insulators represent a relatively recent discovery of a state of matter defined by the topology of the material's electronic band structure rather than a spontaneously broken symmetry. What is unique about this particular state is that unlike the quantum Hall state—which is also characterized by a topology,—it can exist at ambient conditions: room temperature and zero magnetic field. In general, discovering, understanding, and experimentally demonstrating novel phases of matter in strongly correlated systems will lay a foundation for new technological paradigms. Nanometer-scale physics, often interpreted as a separate field, is also of interest as confined geometries and reduced dimensionality enhance interactions between electrons leading to unusual many-body effects. A critical component for gaining new insights is the development of unique instrumentation and this program supports the construction and demonstration of new methods for probing and *controlling* unique quantum phenomena.

3. Optical Physics and Fields. The goal of this Program Area is to explore the formation of light in extreme conditions and the novel manipulation of light. Research is focused on physical regimes where the operational physics deviates dramatically from what is known. The specific research thrusts within this Program Area are: (i) Extreme Light and (ii) Meta-optics. The Extreme Light thrust involves investigations of ultra-high intensity light, light filamentation, and femtosecond/attosecond laser physics. High-energy ultrashort pulsed lasers have achieved intensities of 10^{22} W/cm^2. Theoretical and experimental research is needed to describe and understand how matter behaves under these conditions, including radiation reactions and spin effects, from single particle motion to the effects in materials, and how to generate these pulses and use them effectively. One consequence of ultra-high power lasers is light filamentation. Short, intense pulses self-focus in the atmosphere until the intensity reaches the breakdown value where nitrogen and oxygen are ionized, creating a plasma. This new form of radiation creates a supercontinuum of coherent light across the visible spectrum. Ultra-short intense pulses can be utilized to develop attosecond pulses by combining them with high harmonic generation. Potential long-term applications of these pulses include imaging through opaque materials, laser pulse modulation, "observing" electron dynamics, and even controlling electron dynamics. Research in the Meta-optics thrust includes studies of optical angular momentum (OAM) beams, interactions with metamaterials, and novel optical physics. An example is the study of OAM beams and how they interact with metamaterials, or how they can be used to induce new kinds of interactions or physics. Another area of interest regards overcoming losses in metamaterials. Cloaking is a well-known idea, but losses and the dispersion must be overcome before this is a reality in the practical sense. In addition, other fields which may be used in place of electrodynamics are of interest to this program. Examination of parity-time symmetric optics is being considered as a means to understand and compensate for loss, and topological photonics, calculation of the Chern number, and topological interactions are of interest.

4. Quantum Information Science. The objective of this Program Area is to understand, control, and exploit nonclassical, quantum phenomena for revolutionary advances in computation, sensing and secure communications. Three major Thrusts are established within this program: (i) Foundational Studies, (ii) Quantum Computation and Communication, and (iii) Quantum Sensing and Metrology. Research in the Foundational Studies Thrust involves experimental investigations of the wave nature of matter, including coherence properties, decoherence mechanisms, decoherence mitigation, entanglement, nondestructive measurement, complex quantum state manipulation, and quantum feedback. The objective is to ascertain current limits in creating, controlling, and utilizing information encoded in quantum systems in the presence of noise. Of particular interest is the demonstration of the ability to manipulate quantum coherent states on time scales much faster than the decoherence time, especially in systems where scalability to many quantum bits and quantum operations is promising. Quantum Computation and Communication entails experimental demonstrations of quantum logic performed on several quantum bits operating simultaneously. Demonstrations of quantum feedback and error correction for multiple quantum bit systems are also of interest. There is particular interest in developing quantum algorithms for solving NP-complete problems for use in resource optimization and in developing quantum algorithms to simulate complex physical systems. Research in the Quantum Sensing and Metrology Thrust involves studying the transmission of information through quantum entanglement, distributed between spatially separated quantum entities. Long-range quantum entanglement, entanglement transfer among different quantum systems, and long-term quantum memory are of interest. An emerging field of interest is quantum sensing and metrology using small entangled systems. Entanglement provides a means of exceeding classical limits in sensing and metrology and the goal is to demonstrate this experimentally.

C. Research Investment

The total funds managed by the ARO Physics Division for FY15 were $51.1 million. These funds were provided by multiple funding sources and applied to a variety of Program Areas, as described here.

The FY15 ARO Core (BH57) program funding allotment for this Division was $7.9 million, which included a non-recurring annual increase of $0.9 million. The DoD Multi-disciplinary University Research Initiative (MURI), the Defense University Research Instrumentation Program (DURIP), and the Presidential Early Career Award for Scientists and Engineers (PECASE) program provided $10.0 million to projects managed by the Division. The Division also managed $3.0 million of Defense Advanced Research Projects Agency (DARPA) programs, and $27.6 million provided by other DoD agencies. The Small Business Innovative Research (SBIR) and Small Business Technology Transfer (STTR) programs provided $0.8 million for contracts. Finally, $1.9 million was provided for awards in the Historically Black Colleges and Universities and Minority Institutions (HBCU/MI) Programs, which includes $0.1 million of ARO Core (BH57) funds, in addition to funding for DoD-funded Partnership in Research Transition (PIRT) and DoD-funded Research and Educational Program (REP) projects.

II. RESEARCH PROGRAMS

ARO participates in the creation, leadership, and management of research programs that are supported with funds from a variety of DoD sources. For a detailed description of the purposes and goals for each of these programs, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. Unless otherwise noted, the following sub-sections identify the research awards managed by this Division that began in FY15 (*i.e.*, "new starts"), categorized by program type.

A. ARO Core (BH57) Program

As discussed in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the Army provides funds for the ARO Core (BH57) Research Program. The primary goal of the Core Program is to support high-risk, high-payoff basic research. Research opportunities are identified by a variety of means, including discussions with potential investigators, which may lead to white papers and proposal submissions. Proposals are selected for funding within each ARO Division (*i.e.*, scientific discipline) that take advantage of scientific opportunities that address Army needs and interests with long-term, high-risk ideas. These funds constitute a key mechanism for the Army's support of fundamental research.

The following subsections summarize projects awarded in FY15 and managed by the Division, organized according to the five Core Program categories. Selected projects are discussed in detail later in this chapter (see Sections III-V), with a focus on recent scientific accomplishments, technology transitions, and anticipated accomplishments.

1. Single Investigator (SI) Program. In FY15, the Division awarded 15 new-start SI fundamental research projects, in addition to active awards continuing from prior years. The following principal investigators (PIs) and corresponding organizations were recipients of new-start SI awards.

- Professor Alan Aspuru-Guzik, Harvard University; *Quantum Computation and Communication*
- Professor Gaurav Bahl, University of Illinois - Urbana-Champaign; *Engineered photonic crystals for spontaneous Raman laser cooling in silicon*
- Professor Cheng Chin, University of Chicago; *Experiments with Quantum Matter Synthesizer*
- Professor Liang Feng, State University of New York - Buffalo; *Parity-Time Photonic Synthetic Media: From Nonlinear and Singular Optics to Lasing*
- Professor Nuh Gedik, Massachusetts Institute of Technology; *Realizing Novel Phases of Materials with Light-Matter Interaction*
- Professor Zoran Hadzibabic, University of Cambridge; *Equilibrium and Non-equilibrium Condensation Phenomena in a Tuneable Homogeneous Bose Gas*
- Professor Joseph Haus, University of Dayton; *Nonlinear Optical Signatures of Electronic Quantum Tunneling Effects in Nanoplasmonic Systems*
- Professor Eric Hudson, University of California - Los Angeles; *Efficient Cold Molecular Ion Production For the Study of Quantum Coherence and Dipolar Interactions in a Molecular Ion Trap*
- Professor Natalia Litchinitser, State University of New York - Buffalo; *Novel Materials and Structures for Nonlinear Optics*
- Professor Steven May, Drexel University; *New Routes for Structural, Orbital, and Magnetic Control in Isovalent Oxide Superlattices*
- Professor Alex Retzker, Hebrew University of Jerusalem; *A Novel Ultrafast Pulse Platform for Quantum Technology*
- Professor David Snoke, University of Pittsburgh; *Exciton-Photon Transfer and the Electrical Transport Properties of Polariton Condensates*
- Professor Hakan Tureci, Princeton University; *Stabilizing Quantum Information through Dissipation*

- Professor Jigang Wang, Iowa State University of Science and Technology; *Non-Equilibrium Quantum Phase Discovery via Non-thermal Ultrafast Quench near Quantum Critical Points*
- Professor Amir Yacoby, Harvard University; *Exploring New Approaches for Coupling Spin Qubits*

2. Short Term Innovative Research (STIR) Program. In FY15, the Division awarded five new STIR projects to explore high-risk, initial proof-of-concept ideas. The following PIs and corresponding organizations were recipients of new-start STIR awards.

- Professor Richard Averitt, University of California - San Diego; *Conductivity Dynamics of the Metal to Insulator Transition in $EuNiO_3/LANiO_3$ Superlattices*
- Professor John Howell, University of Rochester; *Cold Atoms and Nanocrystals in Tapered Nanofiber and High-Q Resonator Potentials*
- Professor Benjamin Lev, Stanford University; *Characterizing a Multimode Cavity QED System*
- Professor Max Tegmark, Theiss Research; *Improved Algorithms for Quantifying Integration in Physical Systems Processing Information*
- Professor Jigang Wang, Iowa State University of Science and Technology; *Ultrafast Non-equilibrium Probes of Quantum Critical Regions in Doped $BaFe_2As_2$ via Terahertz Non-Adiabatic Quantum Quench*

3. Young Investigator Program (YIP). In FY15, the Division awarded two new YIP projects to drive fundamental research in areas relevant to the current and future Army. The following PIs and corresponding organizations were recipients of the new-start YIP awards.

- Professor Alexander Gray, Temple University; *Controlling Fundamental Physical Interactions in Strongly-Correlated and Two-Dimensional Electronic Systems with Ultrafast THz Electric Fields*
- Professor James Rondinelli, Northwestern University Evanston Campus; *Ab initio Design of Noncentrosymmetric Metals: Crystal Engineering in Oxide Heterostructures*

4. Conferences, Workshops, and Symposia Support Program. The following scientific conferences, workshops, or symposia were held in FY15 and were supported by the Division. This support was provided via competitive grants to academic researchers responsible for organizing or leading scientific conferences.

- *Quantum Networking Conference: Workshop for Quantum Repeaters and Networks*; Asilomar Conference Grounds Pacific Grove, CA; 15 May - 17 May 2015
- *46th American Physical Society Division of Atomic, Molecular, and Optical Physics*; Columbus, Ohio; 8-12 June 2015
- *Parafermion*; Research Triangle Park, NC; 19-20 August 2015
- *International Conference Bose-Einstein Condensation 2015*; Sant Feliu de Guíxols, Spain; 5-11 September 2015
- *Workshop on Potential Future Directions in Physics*; Research Triangle Park, NC; 16-17 September 2015
- *Nonlinear Metamaterials Incubator*; Washington, DC; 30 September – 2 October 2015

5. Special Programs. In FY15, the ARO Core Research Program provided approximately half of the funds for all active HBCU/MI Core Program projects (refer to CHAPTER 2, Section IX). The Division also awarded five new High School Apprenticeship Program (HSAP) / Undergraduate Research Apprenticeship Program (URAP) grants to support summer research efforts by promising high school or undergraduate students, to be completed at academic laboratories in conjunction with active Core Program awards (refer to CHAPTER 2, Section X).

B. Multidisciplinary University Research Initiative (MURI)

The MURI program is a multi-agency DoD program that supports research teams whose efforts intersect more than one traditional scientific and engineering discipline. The unique goals of the MURI program are described in detail in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. These projects constitute a significant portion of the basic research programs managed by the Division; therefore, all of the Division's active MURIs are described in this section.

1. Conversion of Quantum Information among Platforms. This MURI began in FY09 and was awarded to a team led by Professor Christopher Monroe at the University of Maryland. The objective of this MURI is to explore the conversion of quantum information from one form to another.

Since the inception of research in quantum information, a number of platforms have been explored to implement quantum information: trapped ions, ultracold atomic gases, semiconductor quantum dots, superconductors, and others. Each of these systems has a unique advantage while also suffering disadvantages in other areas. For example, trapped ions are relatively easy to manipulate and are readily isolated from the environment. However they cannot be readily scaled up to the size necessary for practical applications. Semiconductors are perfect for that, but the quantum information is too quickly lost to the surrounding material for a practical computation to occur. To address these matters, the MURI is considering the potential for converting quantum information from one platform to the other without losing the quantum nature of the information. In particular the intra-conversion of information between atomic systems, solid state systems, and optical systems is being explored. If the best of each platform can be combined and the detrimental problems avoided, then the development of quantum information capabilities will be accelerated. The advent of a quantum computer will provide solutions to problems that are computationally intractable on conventional computers, impacting resource optimization and improved logistical support.

2. Harnessing Electronic Phenomena at Oxide Interfaces. This MURI began in FY09 and was awarded to a team led by Professor Susanne Stemmer at the University of California - Santa Barbara. The objective of this research is to investigate the unexpected electronic effects found to exist at the interfaces of certain crystalline oxides.

Recent studies have shown that carefully designed and grown interfaces between different crystalline oxides can lead to electronic phenomena at that interface that are foreign to the oxides that form it. These studies have suggested the potential for a new type of electronics technology; therefore this new MURI aims to determine if these effects can be designed and controlled. The research focuses on the Mott transition: a metal-to-insulator transition that results from electron-electron repulsion. The objective is to design and control the oxide-oxide interface as a new approach to understanding, predicting and controlling the Mott metal-insulator transition and the associated electronic phenomena. The electronic energy states that determine the character of the material are tied to the metal-oxygen atom distance in the crystal and the crystal symmetries. Accordingly the team will construct alternating layers of a material containing a known Mott metal-insulator transition with an insulator that will affect the bonding distances and symmetry of the adjacent Mott material. The ability to control this transition may lead to new options for enhancing logic, memory and other technologies important for advanced computational capabilities.

3. Transformation Optics - Exploring New Frontiers in Optics. This MURI began in FY09 and was awarded to a team led by Professor David Smith at Duke University. The objective of this research is to explore new frontiers in optics made possible by the discovery of negative-index materials (NIMs).

In current optics technology, light refracts (bends) as it passes from one material to another. By curving a surface, such as a lens, refraction is used to focus light. Unfortunately this process loses some of the information contained within the light. As a result, current lenses, such as those used in a microscope, essentially prevent the user from viewing objects smaller than the wavelength of visible light (*i.e.*, limited to about 0.5 micrometers). NIMs can be designed through the use of metamaterials (*i.e.*, artificial materials engineered to provide specific properties not available in naturally-made structures) or by the construction of photonic crystals.

A prior MURI award (FY06-FY11) that was managed by the ARO Physics Division and led by Professor Vlad Shalaev at Purdue University, pioneered many early discoveries and advances in NIMs that in turn manifested a new field in optics termed transformation optics. By combining the negative refraction of NIMs with an index of refraction that varies spatially and temporally, optical materials can be designed to have properties not possible with conventional optics. This MURI team, which includes Professor Shalaev as a co-investigator, is exploring this new frontier in physics. The researchers are investigating methods of controlling light by design, routing it where conventional optics cannot. For example, with transformation optics, light of a particular wavelength can be bent around an object rendering the object invisible at that wavelength. This has already been demonstrated in the microwave band but has not yet been shown at the wavelengths of visible light. The second objective is the development of a flat hyperlens: a lens that is flat on both sides and not only magnifies but also resolves nanometer-scale features. This lens could provide a resolution at least an order of magnitude beyond the diffraction limit of conventional optics. Not only can transformation optics be used to bend light around an object but it can also be used to bend light toward an object. The third major objective is to design materials accordingly such that light from all directions is concentrated on a single detector. These concentrators could revolutionize optical sensors and solar energy collection as its omnidirectional nature eliminates the requirement of moving parts.

4. Atomtronics: an Atom-Analog of Electronics. This MURI began in FY10 and was awarded to a team led by Professor Ian Spielman of the University of Maryland. The objective of this MURI is to explore and understand the concepts of atom-based physics, beginning with the rich and fundamental physics discoveries already revealed with cold atoms systems and to investigate the concepts required for future device applications.

Atom-based physics studies (atomtronics) are analogous to, but will go beyond, the fundamental twentieth century studies regarding the properties of electrons (*i.e.*, electronics) that enabled the electronics revolution. Solid-state electronics, heralded by the transistor, transformed both civilian and military culture within a generation. Yet there is only a single kind of electron: its mass, charge and spin (and thus quantum statistics as well) are unalterable. Atoms on the other hand, come with different masses, can have multiple charge states, and have a variety of spin and other internal quantum states. Accordingly, studies in atomtronics aim to understand an atom-based physics rather than electron-based device physics. Breakthroughs in cold atom physics and degenerate quantum gases presage this new kind of device physics. That cold atom science has resulted in atomic analogies to other technologies, such as optics and lasers, suggests that the same may be repeated with electronics. Very good analogies of solids and junctions can be made with trapped atoms. It is now well-known how one, two and three dimensional structures with essentially any lattice geometry can be formed in cold, trapped atoms. A few theory papers have pointed the way to simple devices.

The most apparent, but not necessarily the only approach to atomtronics, is through optical lattices, where Bloch's theorem holds. Band structure is the first basis on which physicists understand traditional (electronic) metal, insulator, and semiconductor behavior. Interaction and disorder modify this and exploration of Mott-like and Anderson-like insulators and transitions are envisioned as well. Doping can be mimicked by modifying atoms in certain wells or by locally modifying the lattice potential, which can be done with additional optical fields. Such defects could be deeper or shallower wells, or missing or additional sites. Recent breakthroughs involving three dimensional optical lattices and the loading of atoms into lattices with reasonably long lifetimes have set the stage for atomtronics.

Atomtronics researchers are focused on two key themes devices and connections. The envisioned analogs to devices can be described as those that perform actions under external control and those that can be cascaded. The researchers will explore spin-orbit coupling in atomic systems in an effort to exploit new degrees of freedom in "spintomic" device concepts as well as novel reversible logic via cascaded spintomic gates. In addition, researchers will investigate far from equilibrium regimes, which is not possible in condensed matter systems due to the residual phonon interactions at finite temperatures. The second theme centers on connections and is split between analogs to electronics and novel interfacing. The research team use the superfluid properties of ultracold atoms confined in rings to create circuits. These small circuits interact with lasers to demonstrate an analogous SQUID device. Finally the researchers are exploring novel interfacing by trapping atoms with evanescent waves along ultrathin optical fibers. It is hoped that this technique will allow several devices to be coupled while remaining isolated from the environment.

5. Multi-Qubit Enhanced Sensing and Metrology. This MURI began in FY11 and was awarded to a team led by Professor Paola Cappellaro at the Massachusetts Institute of Technology. The objective of this research is to explore and demonstrate imaging, sensing and metrology beyond the classical and standard quantum limits by exploiting entangled multi-qubit systems.

Precision measurements are among the most important applications of quantum physics. Concepts derived from quantum information science (QIS), such as quantum entanglement, have been explored for the past decade to enhance precision measurements in atomic systems with potential applications such as atomic clocks and inertial navigation sensors. QIS has also enabled the development of new types of controlled quantum systems for the realization of solid-state qubits. These systems could potentially be used as quantum measurement devices such as magnetic sensors with a unique combination of sensitivity and spatial resolution. However, progress towards real-world applications of such techniques is currently limited by the fragile nature of quantum superposition states and difficulties in preparation, control and readout of useful quantum states. The power of entangled and squeezed states for quantum sensing lies in their sensitivity to the external parameter to be measured.

This MURI aims to overcome three major obstacles to practical quantum sensor operation: the difficulty to experimentally create desired entangled many-qubit input states to the sensing device, the fragility of the states during signal acquisition, and low fidelity of the readout process. The results of this research may ultimately lead to dramatic improvements in imaging, sensing, and metrology.

6. Light Filamentation. This MURI began in FY11 and was awarded to a team led by Professor Martin Richardson at the University of Central Florida. The objective of this research is to establish the underlying qualitative and quantitative understanding of the physical phenomena associated with light filaments in order to create and control the filaments and their associated unique properties.

A light filament is a novel form of propagating energy that is a combination of a laser beam and plasma. A light filament has three characteristics that make it unlike any other form of energy, and also make it ideal for remote detection of trace materials. Like laser light, a light filament is coherent. However, unlike laser light, it undergoes wavelength dispersion as the beam propagates, creating a coherent beam with wavelengths across the entire visible spectrum. Since the beam contains laser radiation at every wavelength, it is sometimes called a super-continuum or white laser. The continuum has a high UV content, which makes it of interest for remote chemical spectroscopy. Finally, by beating the diffraction limit, a light filament does not diverge in space. Unlike any other form of energy propagation, a light filament can be as small at a distant target as it was when it was created. Light filaments are formed when intense laser pulses are focused down, due to the nonlinearity of the air (the Kerr effect), to about 100 microns. At this point, the intense field ionizes, creating a plasma. The plasma stops the self-focusing and equilibrium is reached. The complex interaction of the plasma and electromagnetic field creates these unique properties of light filaments. Although light filaments are extremely rich in phenomena for potential applications, the complex interaction of optical, plasma, and electromagnetic behaviors is poorly understood.

The research team is attempting to create light filaments and understand and predict light filament propagation characteristics, length, interactions with matter, and electromagnetic interactions. If successful, this research could ultimately lead to controllable light filaments that would revolutionize remote detection and imaging through clouds, creating a new ability in standoff spectroscopic detection.

7. Surface States with Interactions Mediated by Bulk Properties, Defects and Surface Chemistry. This MURI began in FY12 and was awarded to a team led by Professor Robert Cava at Princeton University. This project is exploring the recently-discovered class of materials known as topological insulators.

A topological insulator is a material that behaves as a bulk insulator with a surface that is metallic (permitting the movement of charges on its surface) due to the fundamental topology of the electronic band structure. This topological property separates it from nearly every other known phase of matter. Instead of a phase being due to a broken symmetry (such as results in crystalline, magnetic, superconducting, etc. phases), the property of metallic surfaces results from a transition between two topologically distinct phases: trivial and non-trivial. This is a parallel to the quantum Hall effect which also results from topology but it has two dramatic enhancements. First, it is not limited to two dimensions, and second, the physics should be able to survive to ambient conditions if materials are sufficiently clean. The quantum Hall effect and related phenomena require ultra-low temperatures and high magnetic fields to induce them. Topological insulators do not.

The objective of this research is to advance the discovery, growth, and fabrication of new bulk- and thin-film-based topologically-stabilized electronic states in which electron-electron interactions play a significant role. The researchers are bringing strong materials science, chemistry and surface science approaches to bear on the study of the novel properties of topological insulators. Research in this area has great potential for long-term benefits for the Army, such as electronically-controlled magnetic memory and low-power electronics.

8. High-Resolution Quantum Control of Chemical Reactions. This MURI began in FY12 and was awarded to a team led by Professor David DeMille at Yale University. This MURI is exploring the principles of ultracold molecular reaction, where chemical reactions take place in the sub-millikelvin temperature regime. This research is co-managed by the Chemical Sciences and Physics Divisions.

The study of ultracold molecular reactions, where chemical reactions take place in the sub-millikelvin temperature regime, has emerged as a new field in physics and chemistry. Nanokelvin chemical reactions are radically different than those that occur at "normal" temperatures. Chemical reactions in the ultracold regime can occur across relatively long intermolecular distances, and no longer follow the expected (Boltzmann) energy distribution. The reactions become heavily dependent on nuclear spin orientation, interaction strength, and correlations. These features make them a robust test bed for long-range interacting many-body systems, controlled reactions, and precision measurements.

The objectives of this MURI are to develop a fundamental understanding of the nature of molecular reactions in the nano-K temperature regime and to extend the cooling technique previously demonstrated by Professor DeMille[1] (through a previous ARO award) to other molecular candidates. The researchers are focused on the implementation of novel and efficient laser cooling techniques of diatomic molecules, and to understand the role of quantum effects, including the role of confined geometries, on molecules that possess vanishingly-small amounts of thermal energy. This research could lead to new devices or methods that explicitly use quantum effects in chemistry, such as the precision synthesis of mesoscopic samples of novel compounds, new avenues for detection of trace molecules, and a new understanding of combustion and atmospheric chemical reactions.

9. Non-equilibrium many-body dynamics. This MURI began in FY13 and was awarded to a team led by Professor Cheng Chin at the University of Chicago. The goal of this MURI is to study fundamental non-equilibrium dynamics using cold atoms in optical lattices.

Dynamics far from equilibrium is of great importance in many scientific fields, including materials science, condensed-matter physics, nonlinear optics, chemistry, biology, and biochemistry. Non-equilibrium dynamics recently has taken on significance in atomic physics, where new tools will enable breakthroughs. In particular, optical lattice emulation is allowing one to gain insight, and potentially solve, traditionally intractable problems, including those out of equilibrium. Breakthroughs in other disciplines are also enabling a new look at non-equilibrium. In materials science, a recent pump-probe experiment enabled dynamical control of material properties.[2] Another example is in biochemistry, in determining the role that non-equilibrium phase transitions play in driven biochemical networks, e.g., canonical phosphorylation-dephosporylation systems with feedback that exhibit bi-stability.[3-4] Despite the ubiquitous nature of non-equilibrium dynamics, little scientific progress has been made due to the many challenges, including the difficulty in finding many-body systems that remain far from equilibrium on experimentally accessible time scales.

The objective of this MURI project is to discover how many-body systems thermalize from non-equilibrium initial states, and explore the dynamics of far-from-equilibrium systems. Given that non-equilibrium dynamics plays an important role in many scientific and engineering areas, such as quantum sensing and metrology, atomtronics, and quantum chemistry, this research could ultimately lead to the development of dynamic materials, and devices for improved computation, precision measurement, and sensing.

10. Ultracold Molecular Ion Reactions. This MURI began in FY14 and was awarded to a team led by Professor Eric Hudson at the University of California - Los Angeles. The goal of this MURI is to design, create, and exploit molecular ion traps to explore precision chemical dynamics and enable the quantum control of ultracold chemical reactions. This research is co-managed by the Chemical Sciences Division.

Investments quantum computing and precision metrology have led to the development of molecular ion trap technology. These advances provide scientific opportunities that could be exploited to enable new methods for the study and control of chemical reactions. Recent scientific breakthroughs have been achieved in ultra-cold chemistry with neutrals, suggesting that ion chemistry would provide similar opportunities for an emerging new field. In addition, work in quantum information has led to the development of new types of arrayed micro-fabricated ion traps. Ion trap technology adds novel capabilities to molecular ion research, enabling new

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[1] Shuman ES, Barry JF, DeMille D. (2010). Laser cooling of a diatomic molecule. *Nature*. 467:820–823.

[2] Goulielmakis E, Yakovlev VS, Cavalieri AL, et al. (2007). Attosecond control and measurement: lightwave electronics. *Science*. 317:769-775.

[3] Qian H. (2006). Open-system nonequilibrium steady state: statistical thermodynamics, fluctuations, and chemical oscillations. *J. Phys. Chem. B*. 110:15063-15074.

[4] Ge H and Qian H. (2011). Non-equilibrium phase transition in mesoscopic biochemical systems: from stochastic to nonlinear dynamics and beyond. *J. R. Soc. Interface*. 8:107-116.

research opportunities in materials science, condensed-matter physics, chemistry, and biochemistry. In particular, ion traps offer dramatic improvements in chemical sensing at the single-ion level. Compared with molecular neutrals, trapped molecular ions offer interaction times much longer than what is possible in beam experiments; state preparation and readout is potentially cleaner; and Coulomb interactions with co-trapped atomic ions allow for general species-independent techniques.

The objective of this research is to develop and create molecular ion traps to exploit long interrogation time to study molecular ion chemistry, utilize extended interaction times and dipolar interactions in novel quantum control scenarios, improve chemical sensing using single-ion detection, and integrate the traps with various detectors. This research could ultimately leave to dramatically improved methods for creating and studying quantum dots, energetic compounds, biological reactions, and tools for detection of trace molecules.

11. Engineering Exotic States of Light with Superconducting Circuits. This MURI began in FY15 and was awarded to a team led by Professor Andrew Houck at Princeton University. The goal of this MURI is to initiate significant new experimental and theoretical explorations to harness recent breakthroughs in superconducting systems and to demonstrate useful new states of light that can be brought to bear on broader goals in sensing, measurement, simulation, and computation. This research is co-managed with the Electronics Division. If successful, this research may lead to new tools for metrology, could provide key insight into non-equilibrium quantum systems, and will provide new resources for quantum communication and sensing.

Quantum optics, particularly in the domain of cavity quantum electrodynamics, provides a pathway to create and use large macroscopic quantum states with photons. Such states have been difficult to generate because atoms trapped in a cavity provide only weak nonlinearity to mediate photon-photon interactions, high photon loss introduces decoherence, low photon collection and detection efficiency decrease success probability, among other challenges. On the other hand, recent progress in superconducting qubits and high-quality microwave cavities for quantum computing has enabled orders of magnitude improvements in coherence, fast single shot high-fidelity readout, high-fidelity quantum operations, low photon loss, and better understanding of decoherence mechanisms. These advances have enabled early experiments that have demonstrated the creation of high-fidelity coherent states with several tens of photons. In addition, the new generation of superconducting devices opens up the opportunity for the exploration of new regimes of quantum optics involving quantum states of 100s of photons. Further advances are possible if, in addition to the physics of quantum optics, advanced microwave circuit engineering is brought to bear on the regime of low-power microwave signals to improve coherence and function, and materials science is employed to determine relationships between decoherence and defects in materials, surface chemistry, and interface quality. In turn, the superconducting systems and the quantum states created in them could also be used as sensitive probes of materials behavior, in particular of the origin and sources of decoherence and dissipation mechanisms.

The multidisciplinary research team led by Professor Houck combines the efforts of physicists and engineers who will develop the theoretical and experimental tools to establish new regimes of quantum optics using superconducting circuits. The new states of light established in this program provide new tools for metrology, could provide key insight into non-equilibrium quantum systems, and in the long term may lead to applications in quantum communication and sensing.

C. Small Business Innovation Research (SBIR) – New Starts

No new starts were initiated in FY15.

D. Small Business Technology Transfer (STTR) – New Starts

In contrast to many programs managed by ARO, the STTR program focuses on developing specific applications, as is described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*. In FY15, the Division managed two new-start Phase I SBIR contracts, in addition to active projects continuing from prior years. These contracts aim to bridge fundamental discoveries with potential applications. A list of SBIR topics published in FY15 and a list of prior-year SBIR topics that were selected for contracts are provided in CHAPTER 2, Section VIII.

E. Historically Black Colleges and Universities / Minority Institutions (HBCU/MI) Programs – New Starts

The HBCU/MI and related programs include the (i) ARO (Core) HBCU/MI Program, which is part of the ARO Core BAA, (ii) Partnership in Research Transition (PIRT) Program awards, (iii) DoD Research and Educational Program (REP) awards for HBCU/MI, and (iv) DoD Instrumentation awards for Tribal Colleges and Universities (TCU). In FY15, the Division managed one new ARO (Core) HBCU/MI project and five new REP awards, in addition to active projects continuing from prior years. Refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES* for summaries of new-start projects in these categories.

F. Presidential Early Career Award for Scientists and Engineers (PECASE) – New Starts

The PECASE program provides awards to outstanding young university faculty members to support their research and encourage their teaching and research careers. The PECASE winners for each year are typically announced by the White House at the end of the calendar year. However, the FY13-FY15 PECASE recipients had not yet been announced by the end of FY15. For additional background information regarding this program, refer to *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*.

G. Defense University Research Instrumentation Program (DURIP)

As described in *CHAPTER 2: PROGRAM DESCRIPTIONS AND FUNDING SOURCES*, the DURIP program supports the purchase of research equipment to augment current university capabilities or to develop new capabilities for conducting cutting-edge research relevant to long-term Army needs. In FY15, the Division managed eight new DURIP projects, totaling $2.6 million. The university laboratory equipment purchased with these awards is promoting research in areas of interest to ARO.

H. DARPA Quantum Assisted Sensing and Readout (QuASAR) Program

The goal of this program, co-managed by the Physics Division, is to bring state-of-the-art science of metrology and sensing and combine them with today's technological developments. The program goal is to bridge the gap between the best scientific performance and the appropriate packaging for fielding high-performance working sensors that are relevant to the DoD. This program was motivated in large part by the Physics Division and compliments ARO-supported research in ultracold gases, providing theoretical and experimental synergy to the Core program.

III. SCIENTIFIC ACCOMPLISHMENTS

This section identifies fundamental research discoveries, results, and accomplishments that originated from research funded and/or monitored by the Physics Division.

A. Chiral Electronic Transport Heralds New Topological Physics

Professor N. P. Ong, Princeton University, Single Investigator Award,
and Professor R. Cava, Princeton University, MURI Award

The last several years have witnessed an explosion of developments in the new field of topological electronic states. Topological states of matter differ from other states in that they cannot be classified by the symmetries they break in the way that, for example, crystalline solids break translational symmetry or ferromagnets break rotational symmetry. Rather, topological states are classified by a "topological phase" in which fundamental properties of the system are insensitive to smooth changes in material parameters and remain this way unless the system undergoes a quantum phase transition. Some of the field's latest developments involve explorations of proposed Dirac and Weyl semimetals. A Dirac semimetal (DSM) is a three dimensional analog of graphene, having spin-full linear-dispersed electronic energy bands near the Fermi level in the bulk of a (three dimensional) crystal. Weyl semimetals (WSMs) represent a condensed matter analog of particles from high energy physics that obey the Weyl equation. One can induce a DSM to become a WSM by breaking time reversal or inversion symmetry (but not both) and this development is reflected in the band structure via a splitting of Dirac points in momentum space. Each single Dirac point becomes two Weyl points with opposite spin locking, hence, the points must come in pairs, and, like DSM's, WSM's electronic energy bands are linear-dispersed. The density of states at the point in the Brillion zone where the cones meet is vanishingly small; thus their classification as semimetals. Individually, Weyl points have non-zero Berry curvature and are assigned a "topological charge" or "chirality" which must be opposite for each member of a set of points. A necessity of the pairs of Weyl points is that they be connected in momentum space through surface bands, and these surface bands are unique in that they are distinct arcs that originate at one Weyl point and terminate at the other. The full ramifications of the existence of such surface states is an active area of exploration.

Part of the uniqueness of the Weyl points is that they represent a topologically distinct three-dimensional state whereas all other topological states to date reside in a lower dimension than the material itself. A topological insulator for example is a 3D (2D) material with topologically protected surface (edge) states. One of the consequences of the pairs of Weyl points is that, under specific electromagnetic excitation conditions, a current can flow between them. This is referred to as a chiral current because the current flows between Weyl points of opposite chirality. Its existence is referred to as the "chiral anomaly" because it is a direct analog of the long-standing Adler-Bell-Jackiw anomaly (also called the chiral or triangle anomaly) from high energy physics which describes the $3x10^8$ faster decay rate for neutral pions compared to charged pions. This transport pathway is distinct from the transport through topologically trivial states. While other researchers have experimentally observed an earmark of this type of transport, none of the measurements to date have unambiguously demonstrated this chiral anomaly in a WSM. Dr. Ong, working with the delicate, air-sensitive DSM Na_3Bi in a magnetic field, however, recently demonstrated the existence of the current with characteristics consistent with the prediction of the chiral anomaly. Currently, these observations have no other competing explanations.

More specifically, as a result of the split of the Dirac points along the applied magnetic field into Weyl points, the unique band structure induces electrons in the experiment to flow parallel rather than perpendicular to the external magnetic field. The results show that two remarkable features arise in the magnetoresistance of Na_3Bi during the measurement. First, a large positive magnetoresistance (magnetic field increases resistance) is found when the magnetic and electric fields are perpendicular while a significant negative magnetoresistance (magnetic field decreases resistance) is observed when the fields are parallel (see FIGURE 1). This behavior has not been observed in any previously known material. Second, the magnetoresistance is steered by the direction of the magnetic and electric fields (see FIGURE 2).

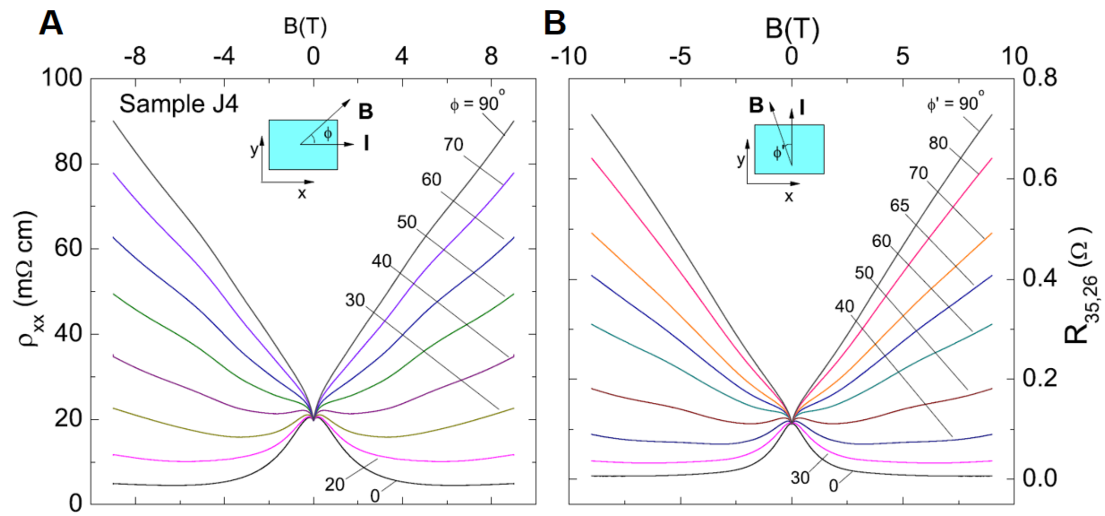

FIGURE 1

Magnetotransport of Na_3Bi relative to current orientation. Magnetotransport was measured for current parallel to the x-axis (**A**) and to the y-axis (**B**) in the a-b plane of the sample. The symmetry of Na_3Bi is C_3 (i.e. hexagonal) so that these directions are fundamentally distinct. In both cases, the magnetic field decreases resistance when the magnetic field is closely aligned to the electric field. This is a strong indication that oft-observed anisotropies in the fermi surface are not responsible for this behavior. Note also that the scattering rate of the chiral current is roughly fifty times less than that of conventional states in zero magnetic field.

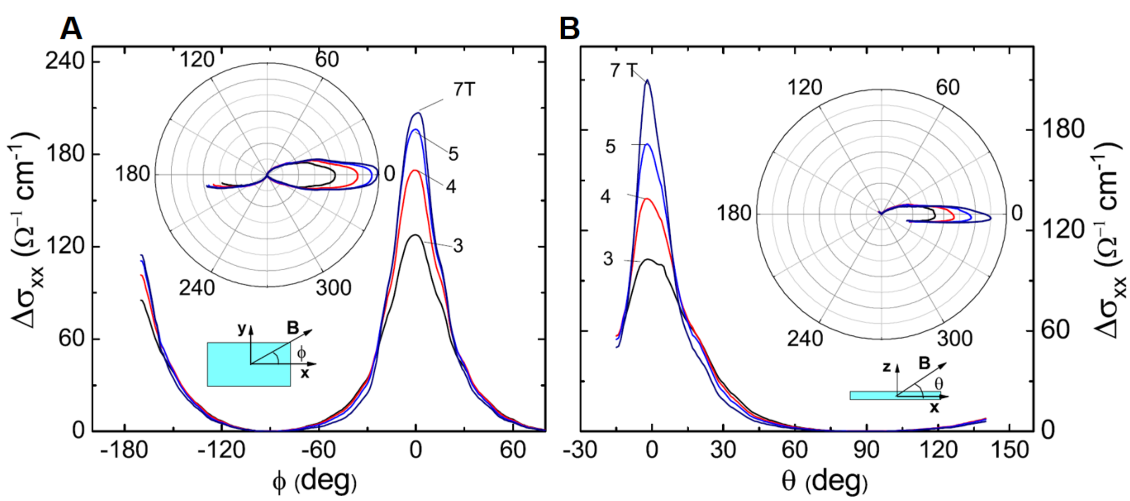

FIGURE 2

Chiral current plume follows the magnetic field. The conductance enhancement is plotted as a function of the angle between the magnetic and electric fields in the (**A**) x-y plane (**B**) x-z plane. The temperature of the sample was 4.5 K for these measurements.

The impact that this discovery will have on condensed matter physics and perhaps eventually electronics is yet to be seen. "Chiral" or "Axial" electronics may provide new technological opportunities. Scientists involved in these studies are currently searching for an ideal material for in-depth exploration of the full ramifications of chiral currents and associated physical effects. In addition to these results, the MURI team theoretically predicted that TaAs is also a Weyl semimetal (without the need for a magnetic field to split Dirac points) and this was experimentally verified within a month of the prediction. Recently, the MURI team has also predicted a second type of Weyl semimetal excitation which has no analog in high energy physics. Among the various families of topological matter, the Weyl semimetals are bound to have prominence.

B. Novel States of Light and Matter Mediated by Collective Rydberg Excitation

Professors Alexey Gorshkov, University of Maryland, and Mikhail Lukin, Harvard University, Single Investigator Award

A grand challenge in quantum optics research is to implement and study strongly interacting photons. In addition to making quantum communication and optical quantum computing more efficient, strongly interacting photons allow for increased precision in imaging and metrology, and also give rise to fascinating many-body physics (e.g. crystallization of photons or novel dissipative time-dependent phenomena). In fact, one could argue that this exciting new direction of many-body physics with strongly interacting photons is the future of quantum optics. One particularly promising approach to achieving strong photon-photon interactions is to use EIT (electromagnetically induced transparency) to couple photons to strongly interacting Rydberg (i.e. highly excited) atoms.

In 2013, ARO funded researchers demonstrated a way to bind two photons together so that one would sit right atop the other, superimposed as they travel. This was the first experimental demonstration and it was considered a major breakthrough because photons usually do not interact with each other.

In September 2015 a paper in *Physical Review Letters* by ARL-ARO supported researchers Alexey Gorshkov from the University of Maryland and Mikhail Lukin from Harvard showed theoretically that by adjusting the parameters of the binding process, photons could travel side by side, a specific distance from each other.[5] The arrangement is akin to the way that two hydrogen atoms sit next to each other in a hydrogen molecule.

Specifically the team showed that two photons coupled to Rydberg states via EIT could interact via an effective Coulomb potential. This interaction gives rise to a continuum of two-body bound states. Within the continuum, metastable bound states are distinguished in analogy with quasibound states tunneling through a potential barrier. The team also found multiple branches of metastable bound states whose energy spectrum is governed by the Coulomb potential, thus obtaining a photonic analogue of the hydrogen atom. Under certain conditions, the wave function resembles that of a diatomic molecule in which the two polaritons are separated by a finite "bond length." These states propagate with a negative group velocity in the medium, allowing for a simple preparation and detection scheme, before they slowly decay to pairs of bound Rydberg atoms (see FIGURE 3).

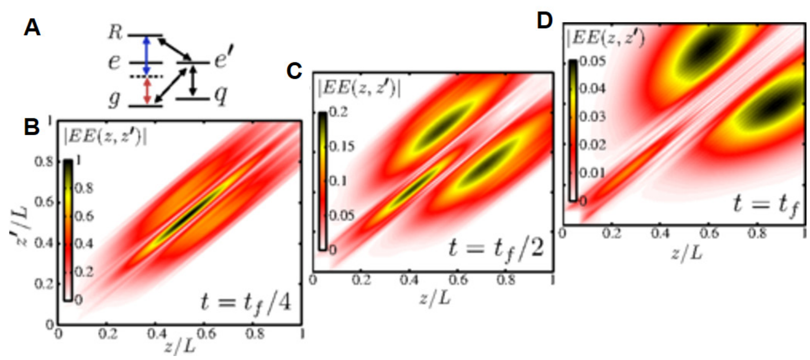

FIGURE 3

Two photons coupled to Rydberg states via EIT interacting via an effective Coulomb potential. (**A**) Level structure used to prepare the initial SS distribution. (**B-D**) Time evolution of a wave packet with all components initially zero except *SS*, which is chosen to be a Gaussian wave packet of variational *n*=1 Coulomb state solutions (with the δ function removed) centered at $\omega = 0$ and having width $\Omega^2/2\Delta$. Specifically, $|EE|$, initially zero, is shown after the initial transient evolution subsides at (**B**) $t = t_f/4$, and at (**C**) $t = t_f/2$ and (**D**) $t = t_f$, where $t_f = 5.5\Delta/\Omega^2$. The wave packet within the blockade radius has the expected shape of the Coulomb state, propagates backward, and decays, while the wave packet outside the blockade radius propagates forward with v_g and disperses. The investigators considered a medium of length $L = 16r_b$, $g^2r_b/c\Delta = 5$, $g/2\pi = 17$ GHz, $\Omega/2\pi = 1.5$ MHz, $r_b = 25$ μm, $\Delta/2\pi = 30$ MHz, $\gamma/2\pi = 3$ MHz, and $\gamma'/2\pi = 5$ kHz.

[5] Maghrebi MF, Gullans MJ, Bienias P, Choi S, Martin I, Firstenberg O, Lukin MD, Büchler HP, and Gorshkov AV. (2015). Coulomb Bound States of Strongly Interacting Photons. *Physical Review Letters.* 115:123601.

"It's not a molecule per se, but you can imagine it as having a similar kind of structure," says NIST's (UMD) Alexey Gorshkov. "We're learning how to build complex states of light that, in turn, can be built into more complex objects. This is the first time anyone has shown how to bind two photons a finite distance apart."

While this work opens the avenue for the creation of Coulomb-like two-photon states, the expectation is that a wide class of both useful and exotic two-photon and multiphoton states can be created via refined engineering of photon-photon interactions, e.g., by using microwave fields. A detailed understanding of the two-photon Rydberg-EIT physics provided by this work also opens up an avenue towards understanding the full—and much richer—many-body problem involving an arbitrary number of photons in any dimension.

C. Probing Molecular Ions with Laser-Cooled Atomic Ions

Professor Kenneth Brown, Georgia Institute of Technology, Single Investigator Award

High precision measurements of molecules and molecular ions are important for studies ranging from fundamental physics to astrochemistry as they often yield insights impossible to gain from atomic systems alone. Expansion of high precision results to a variety of molecular species is challenging, however, due to a dearth of experimental data regarding the frequencies of the transitions. This is due, in part, to the experimental set-ups utilized in high precision measurements often being incompatible with the large scale spectroscopy surveys needed to pinpoint new transition frequencies.

In FY15, Professor Brown's group successfully sought to modify a high precision set-up to identify new molecular transitions by utilizing a chain of laser-cooled Ca^+ atomic ions and one CaH^+ molecular ion in a resonance-enhanced multiphoton dissociation (REMPD) experiment. REMPD is a technique where, depending on an illumination laser being resonant with a transition, a photon can dissociate the molecule under study and induce a fluorescence event. The key development of the FY15 work was driving vibrational overtones of CaH^+ with a ~5 nm bandwidth mode-locked spectroscopy laser capable of spanning CaH^+'s thermally occupied rotational states. This allowed the group to ignore line broadening due to rotational transitions. The experimental scheme is shown in FIGURE 4 along with the final compiled results, where the two newly identified vibrational transitions are visible. This observation is the first measurement of such transitions in CaH^+, shows that single molecular ion experiments can be used to discover new transitions, and demonstrates that experimental set-ups conceived for high precision spectroscopy techniques can be utilized for preliminary large range spectroscopy work. This latter result is important for both fundamental physics research and applications such as single molecule manipulation.

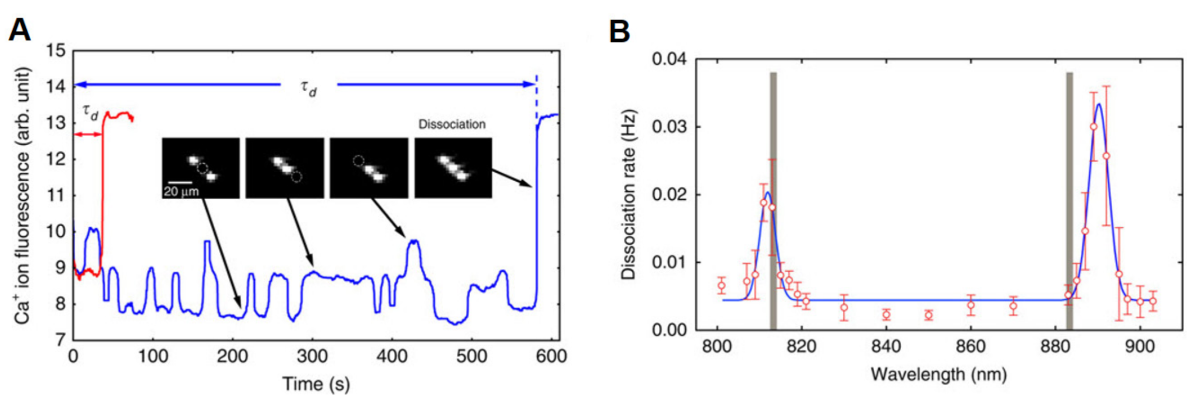

FIGURE 4

Resonance-enhanced multiphoton dissociation results and vibrational overtone spectra from the CaH^+ molecule. (**A**) shows sample fluorescence measurements of a crystal chain of two Ca^+ atomic ions and one CaH^+ molecular ion as a function of time. A dissociation is marked by an increase in fluorescence and indicates that the spectroscopy laser's wavelength is resonant with a vibrational transition of the CaH^+ molecule. The transition strength is inversely proportional to the amount of time it takes for the fluorescence event to appear. The red trace shows an example event where the laser is fully resonant with a vibrational overtone. (**B**) Dissociation rate plotted as a function of the spectroscopy laser's wavelength and clearly indicates two experimentally observed vibrational transitions, one at 812 nm and one at 890 nm. Multiple scans such as those shown in (A) were used to create (B). The disagreement of these wavelengths with predicted theoretical values, shown as gray bars, is in line with previously observed differences between calculated and measured vibrational transitions in other metal hydride systems.

D. From Quantum Computing to Quantum Sensing
Professor Jonathan Dowling, Louisiana State University, Single Investigator Award

Quantum metrology work leveraging number-path entanglement is capable of producing sensors which beat the shot-noise limit, but is non-trivial to implement due to the difficulty inherent in producing number-path entangled states. Recently, however, a new and strikingly simple technique for producing this particular type of entanglement was discovered. Surprisingly, passive, multimode, linear-optical interferometers, fed only with uncorrelated single photon inputs in each mode and subsequently followed by uncorrelated single photon measurements at each output can produce number-path entanglement. Additionally, this entanglement grows superexponentially fast in the resources of mode and photon number. In FY15, Professor Dowling's group began to theoretically investigate if photons entangled using this simple technique, which they call a quantum Fourier transform interferometer (QuFTI), could be successfully leveraged to beat the shot-noise limit (see FIGURE 5). The sensitivities obtained with a QuFTI not only beat the shot noise limit, but beat it by up to a factor of three. Additionally, a comparison with the Heisenberg limit shows that the obtained sensitivities are not far behind. Another advantage of this approach emerged when further work demonstrated that the type of network created using states generated with QuFTI are far more robust against deleterious dephasing than the fragile networks created with the more effort intensive methods.

The ease with which these states are created implies that quantum metrology efforts in gyroscopy, gravimetry, optical coherence tomography, ellipsometry, magnetometry, microscopy, and more can all potentially benefit from enhanced sensitivity. This new approach leveraging easy-to-prepare single-photon states and disjointed photodetection provides a pathway forward to practical quantum metrology with readily available technology.

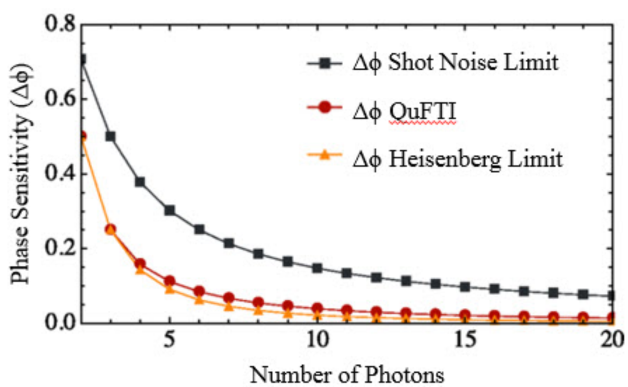

FIGURE 5

QuFTI Sensitivity Comparison. The phase sensitivity vs. the number of photons is shown for three limits discussed in the text: the shot noise, new Quantum Fourier Transform Interferometer (QuFTI), and Heisenberg. The QuFTI technique exhibits a phase sensitivity significantly better than the shot noise limit by up to a factor of three, and is only slightly underperforms compared to the Heisenberg limit.

E. Multi-Qubit Enhanced Sensing and Metrology
Professor Paola Cappellaro, MIT, MURI Award

Magnetic imaging utilizing nitrogen-vacancy (NV) centers in diamond is a powerful and versatile technique providing single electron spin sensitivity and three-dimensional resolution better than 1nm for a variety of physical and biological samples. To obtain this high sensitivity, however, one must utilize slow point-by-point scanning approaches. In FY15 the MURI team lead by Professor Cappellaro devised a microscopy technique for NV centers which bypasses slow real-space imaging and instead utilizes pulsed magnetic field gradients to phase-encode spatial information on NV spins in k-space. This encoding is followed by the use of a fast Fourier transform to ultimately yield real-space images with nanoscale resolution and wide fields of view in a fraction of the time of traditional NV techniques (see FIGURE 6).

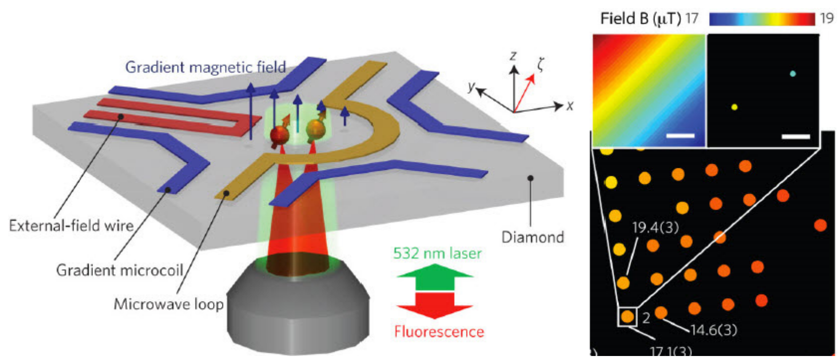

FIGURE 6

Fourier magnetic imaging microscopy. The left side of the figure shows the microscope schematic. NV-center magnetic sensors are located near the surface of a chip and controlled magnetic field gradients for NV spin phase encoding are generated by sending currents through pairs of wires. The right side of the figure illustrates the use of a wide-field, low resolution real space plus high resolution k-space imaging technique capable of obtaining a wide field of view with nanoscale resolution. The lower part of the figure shows the low resolution real space image of a set of nanopillars exposed to a magnetic field gradient. The upper right image shows NV center positions and local magnetic field amplitudes with ~30 nm resolution obtained using the Fourier microscopy technique. The upper left image shows the variation in magnetic field amplitude within a nanopillar obtained with the hybrid technique. This hybrid approach provides a spatial dynamic range (FOV/resolution) of ~500. Additional data proved the microscope capable of one-dimensional NV center imaging with <5 nm resolution, and two-dimensional imaging of nanoscale magnetic field patterns with a gradient sensitivity of ~14 $nT/(nm^{-1}Hz^{-1/2})$. The team also demonstrated that a compressed sensing technique can accelerate the image acquisition time by an order of magnitude.

The novel approach of encoding of information on the NV spins rather than on the spins of the sample under study as is traditionally done in Fourier magnetic imaging opens the technique to imaging a wider variety of nanoscale magnetic phenomena in physical systems than existing Fourier magnetic imaging allows. Possible examples include probing quantum effects in materials such as frustrated magnetic systems with skyrmionic ordering, spin liquids where quantum spin fluctuations prevent the system from ordering, and topological insulators with quantized spin-carrying surface states. In the biology, this technique could allow for nanoscale NMR spectroscopy and real-time non-invasive mapping of functional activity in neuronal networks with synapse-scale resolution (~10 nm) and circuit-scale FOV (>1 mm). These possibilities, along with anticipated technical improvements which should allow sub-1 nm resolution and measurement extensions to include electric field, temperature, and pressure, will only increase the value of this novel Fourier sensing approach.

F. Nonlinear Optical Signatures of Electronic Quantum Tunneling Effects in Nanoplasmonic Systems

Professor Joseph W. Haus, University of Dayton, Single Investigator Award

Professor Haus, along with colleagues Professors Andrew Sarangan and Imad Agha, University of Dayton, Dayton, and Professor Parag Banerjee, Washington University, are studying nanoantennas and a connection between their electromagnetic and electronic quantum tunneling characteristics. The nanoantennas fabricated from different metals and separated by a thin insulator function as rectennas, i.e. antennas that rectify the ac current flowing through them (see FIGURE 7). Rectenna diode characteristics in the Radio Frequency regime have been demonstrated many years ago. The optical and infrared regimes pose challenges, but the payoff can be high, since better than 50% energy harvesting efficiency is predicted.[6] In other words, this revolutionary technology comes with the high-risk of exploratory research. Their design of optical nanorectennas eliminates the need for separate antenna and diode elements. They can be integrated with efficient power management and storage circuits to drive a multitude of electronics/sensors. The academic institutes, the University of Dayton (UD) and Washington University in St. Louis (WUStL), are working with complementary experimental approaches to synthesizing nanoscale structures and validating the underlying physics and establishing their true performance.

[6] Moddel G, Grover S, Eds. (2013) *Rectenna Solar Cells.* Springer, New York.

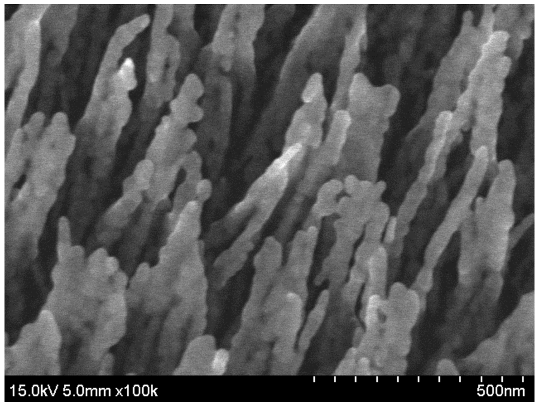

FIGURE 7

A forest of silver nanocolumns grown by glancing angle deposition at cryogenic temperatures.

The research team has been applying a comprehensive quantum theory to understand the fundamental problems on the Angstrom scale called the Quantum Conductivity Theory (QCT) that was collaboratively developed by the PI and Scalora's group at AMRDEC.[7] The validation and device functionalization experiments will be guided by advanced electromagnetic simulations. Contrasted against the classical theory, the quantum theory reduces and quenches the enhancement for small gaps and moreover, the enhancement is further reduced at higher intensities (see FIGURE 8). The UD and WUStL team are working to develop new prototype device designs based on a nanorod geometry and will examine their ultra-broadband lightwave response of the prototype devices. Initial calculations on nanorod antennas will help to guide their experimental studies; to be accurate they are undertaking comprehensive simulations of the linear and nonlinear effects in the materials.[8-9]

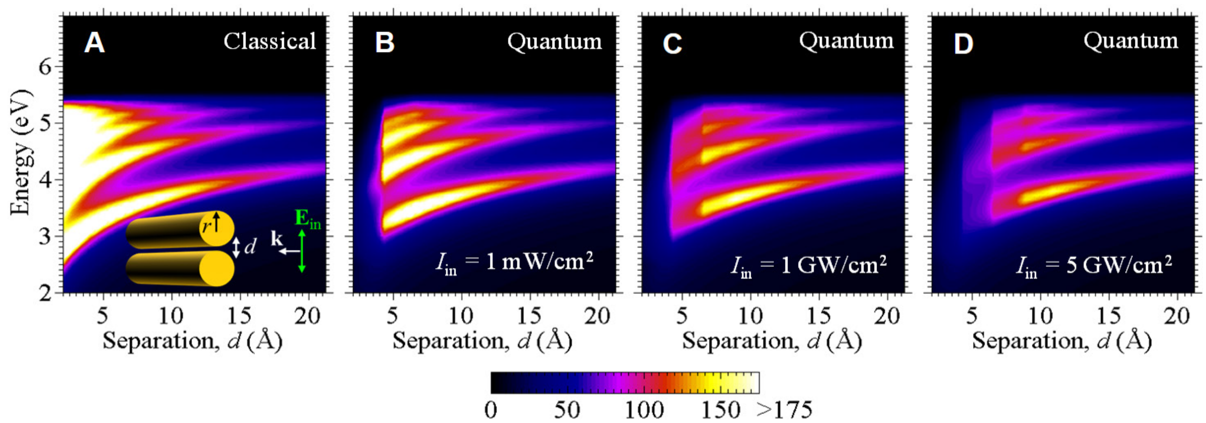

FIGURE 8

Field enhancement at the center of the gap for Au dimers immersed in vacuum using QCT. Considering two parallel, Au cylinders assumed to be infinitely long, with variable separation *d* and radius *r= 4.9 nm*; (**A**) Field enhancement using classical plasmonic theory; (**B**) Field enhancement using QCT in the low irradiance regime (1 mW/cm^2); (**C**) Field enhancement including the nonlinear quantum conductivity in QCT. The irradiance is (C) 1 GW/cm^2 and (**D**) 5 GW/cm^2. The field is TM-polarized, as indicated in the inset in (A).

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7 Haus JW, de Ceglia D, Vincenti MA, Scalora M. (2014). Nonlinear Quantum Tunneling Effects in Nano-Plasmonic Environments. *J. Opt. Soc. Am.* B31,A13

8 de Ceglia D, Vincenti MA, De Angelis C, Locatelli A, Haus JW, Scalora M. (2015). Second harmonic generation from dipole nanoantennas: Role of antenna modes and field enhancement. *Optics Express*. 23:1715-1729.

9 Scalora M, Vincenti MA, de Ceglia D, Cojocaru CM, Grande M, Haus JW. (2015). Nonlinear Duffing oscillator model for third harmonic generation. *J. Opt. Soc. Am. B* 32:2129-2138.

Validation experiments are designed to measure the second-harmonic and third-harmonic signals from metal-insulator-metal (MIM) structures. Their experiments seek to find a quantum tunneling signature in the nonlinear harmonics that can be several orders of magnitude larger than the intrinsic material nonlinearities.[10] These experiments will be the first to critically compare measurements with electromagnetic scattering calculations including nonlocal effects and electronic quantum tunneling phenomena. The first experiments will be fundamental in nature and involve studies on nanoparticles deposited on an ALD-coated surface as a prototype systems allowing us to implement the detection setup and test it. Nanorod samples are then fabricated at UD covering a substrate with metal pillars grown using glancing angle deposition techniques. A few-Å thick alumina (Al_2O_3) or titania (TiO_2) insulator is deposited over the metal pillars using atomic layer deposition and second metal nanocolumn is grown over the first one.

WUStL's fabrication approach uses an anodic alumina template (AAT) to fabricate self-assembled, independent units of single MIM nanorods with Au nanorods, 200 nm in height and 80 nm in diameter are grown in the nanoholes via electrochemical deposition (see FIGURE 9). The density of the nanorods is 10^{10}/cm^{-2}. Within the templates atomic layer deposited (ALD) dielectric films will be deposited, separating the two metallic rods by a few Å spacer layer. The superb control over nanodimensions, aspect ratio and materials already demonstrated by Banerjee's group is evident in the figure. Experiments are in progress to determine the electrical and optical characteristics of MIM diodes.

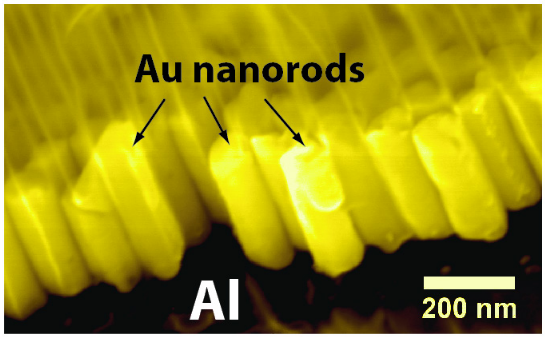

FIGURE 9

Au nanorods 200 nm height, 80 nm diameter grown within AAT. The AAT has been etched away leaving behind the Au nanorods. Rod density is 10^{10}/cm^{-2}.

[10] Scalora M, de Ceglia D, Vincenti MA, Haus JW. (2014). Nonlocal and Quantum Tunneling Contributions to Harmonic Generation in Nanostructures: Electron Cloud Screening Effects. *Phys. Rev.* A90:013831.

IV. TECHNOLOGY TRANSFER

ARO Scientific Divisions seek to identify promising scientific breakthroughs and facilitate the transition of cutting-edge research concepts and data to potential applications. This section describes basic research results, observations, and/or theories that transitioned elsewhere in ARL and/or to external organizations and customers.

A. Josephson Parametric Amplifiers: From Cryogenic Qubits to Commercial Low-Noise Amplifiers

Investigator: Professor Irfan Siddiqi, University of California - Berkeley, Single Investigator
Recipient: Industry

Professor Siddiqi commenced his work with the objective of exploring and developing superconducting Josephson parametric amplifiers to enable single-shot non-demolition readout of cryogenic solid-state qubits. A key obstacle to obtaining single shot fidelity in a quantum state measurement is that dispersive measurements are least perturbative when only a few photons are used, necessitating the use of an amplifiers more sensitive than those readily available. The goals of Professor Siddiqi's group were to produce a standalone 4-8 GHz amplifier with more than 20 dB of gain and larger than 10 MHz bandwidth. Additionally, the amplifier would be integrated on-chip for qubit readout without the need for circulators.

As this work progressed, it drew the attention of Hypres, a digital superconductor company, and they were subsequently selected for a STTR Phase I contract, and then later STTR Phase II funds to transition of Professor Siddiqi's superconducting parametric amplifier work into a product line focusing on three types of low-noise amplifiers in compact cryogenic microwave packages. Hypres' primary focus is directed toward the quantum information community as they develop systems capable of real-time measurements of quantum circuits, but they are also working on broader cryogenic detection systems leveraging the technology. The STTR I work produced a compact package for lumped-element Josephson parametric amplifiers and established the feasibility of digitization of the amplified output of qubits with a superconductor analog-to-digital converter chip. The new STTR II funds will enable the continuation of the work.

V. ANTICIPATED ACCOMPLISHMENTS

The nature of basic research makes it difficult to predict a timeline for scientific discovery; however, ARO-funded research is often on the verge of important achievements. This section describes selected scientific accomplishments predicted to emerge during the next fiscal year.

A. Raman sideband cooling of Silicon

Professor Guarav Bahl, University of Illinois at Urbana-Champaign, Single Investigator Award

During the last two decades anti-Stokes fluorescence cooling of solid state materials has been well established as a novel approach to refrigeration that does not involve mechanical aspects. Recently, this has been demonstrated to cool a macroscopic sample from room temperature to a base temperature below 100 K by illuminating it with a precisely tuned infrared laser. This low temperature is well below what is currently possible with thermoelectric devices and provides an alternative to all solid state cooling. An interesting advantage is that heat is removed optically – no heat sinks or other hardware is needed to move it away from the source or sample. To date, this has been done using glasses doped with rare-earth elements. The materials options and applicability of the technique is limited, however, because the quantum efficiencies of the involved transition processes for fluorescence usually favor Stokes (heating) over anti-Stokes processes. In FY15, Professor Bahl proposed using Raman sidebands instead. As Raman cooling processes are materials independent, this would greatly enlarge the library of materials that could be cooled with lasers. This has not been previously considered because Raman processes favor the Stokes process – adding energy and heating up the sample – over the anti-Stokes process which would take energy away. Using a carefully designed photonic crystal, Professor Bahl aims to suppress the Stokes process and enhance the anti-Stokes process and outlined the procedure in a recent theoretical paper. He found that silicon is an ideal material to cool with Raman anti-Stokes cooling. Professor Bahl is expecting to test this experimentally in FY16. If he is successful, it may strongly impact the technological field of solid state cooling as well as provide the Army with small-scale cooling techniques for electronic technologies.

B. Development of Microwave Ion Chip Entanglement Architectures for Quantum Technologies

Professor Winfried Hensinger, University of Sussex, Single Investigator Award

The objective of Professor Hensinger's project is to explore methods to perform high-fidelity quantum logic and quantum control with trapped ions using microwaves in custom microfabricated ion-trap chips with innovative chip designs. This is a departure from the conventional, laser based, trapped ion manipulation approach and is motivated by attempting to avoid the challenges associated with lasers ranging from inherent frequency, phase, and intensity instability to insufficient power to difficult laser-single ion alignments. Year one of the work was extremely successful and the group has already demonstrated entanglement gate fidelities in excess of 95%. They have also shown conclusively that fault-tolerant gate operations are possible using their static gradient microwave scheme. In the coming year, one primary focus will be to alter the microwave and radio-frequency setup to allow for faster entanglement gate times and increased coherence time of the group's dressed state qubit. Their new configuration will permit pulse shaping and reduce noise and the anticipated results include two-ion gate fidelities much higher than their current ~95%. Additionally, year one work focused on a collaboration with ARL to further innovate ion-chip design has been fruitful and year two should see an acceleration of this portion of the project aimed at increasing the fidelity of microwave gates to even higher levels.

VI. SCIENTIFIC AND ADMINISTRATIVE STAFF

A. Division Scientists

Dr. Marc Ulrich
Division Chief
Program Manager, Condensed Matter Physics

Dr. Richard Hammond
Program Manager, Optical Physics and Fields

Dr. Paul Baker
Program Manager, Atomic and Molecular Physics

Dr. T. R. Govindan (NASA)
Program Manager, Quantum Information Science

B. Directorate Scientists

Dr. Douglas Kiserow
Director, Physical Sciences Directorate

Dr. Peter Reynolds
Senior Scientist, Physical Sciences Directorate

Dr. J. Aura Gimm
Program Manager, Institute for Soldier Nanotechnologies and Institute for Collaborative Biotechnologies

Dr. Kelby Kizer
Special Assistant to the Directorate Director

Dr. Larry Russell, Jr.
International Research Program Coordinator

Mr. John McConville
Technology Transfer Officer, Institute for Soldier Nanotechnologies

C. Administrative Staff

Ms. Inez Kendall
Contract Support

Ms. Wanda Lawrence
Contract Support

Phone: (919) 549-0641

Fax: (919) 549-4310

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