

Fact Sheet: Progress on Materials Genome Initiative May 14, 2012

President Obama announced the <u>Materials Genome Initiative</u> (MGI) on June 24, 2011 with the aim of doubling the speed and reducing the cost of discovering, developing, and deploying new advanced materials. "The invention of silicon circuits and lithium ion batteries made computers and iPods and iPads possible, but it took years to get those technologies from the drawing board to the market place," the President said at Carnegie Mellon University. "We can do it faster."

Indeed, today, it can take 20 years or more for a newly discovered material to be incorporated into commercial products. This pace is far too slow given the range of urgent challenges that high-tech materials can help address, including making vehicles safer and lighter; creating packaging that keeps food fresher and more nutritious; and producing lightweight, bullet-proof vests for law enforcement officers and soldiers. New materials are also a major part of the American manufacturing enterprise—a central feature of the Nation's economy that generates innovation, opportunities, and jobs.

The MGI, announced in conjunction with the Administration's <u>Advanced Manufacturing</u> <u>Partnership</u>, is a multi-agency effort to catalyze a new era of policies, resources, and infrastructure that support American institutions as they work to set a new pace for bringing new materials to market. Already, the Administration has announced investments in nine Federal programs at the Department of Energy, Department of Defense, National Institute of Standards and Technology and National Science Foundation that will support the MGI.

In fiscal year 2012 alone, MGI commitments include:

- \$12 million of research at the **Department of Energy** that will combine computational tools, experimental tools, and digital data to develop and advance high-tech, high-performing materials;
- \$17 million in materials research at the **Department of Defense**, including research to improve the prediction and optimization of materials properties;
- the launch of **National Science Foundation's** Designing Materials to Revolutionize and Engineer our Future with expected awards to be made in summer 2012; and,
- efforts at the **National Institute for Standards and Technology** (NIST) to develop new techniques, standards, and tools for the broader research community, .

But achieving the MGI vision demands an "all hands on deck" approach, with dedicated involvement of academic institutions, small businesses, large industrial enterprises, professional societies, as well as government. Toward that end, on May 14, 2012, a number of businesses and universities announced new commitments to advance the MGI.

NEW COMMITMENTS BY INDUSTRY AND UNIVERSITIES

Harvard to Release 7 Million New Materials Leveraging IBM's World Community Grid and a Partnership with Wolfram Research

In one of the largest computational chemistry experiments in history, <u>The Clean Energy Project</u>, led by the Aspuru-Guzik group at Harvard University, is using IBM's World Community Grid to accelerate the testing of millions of new, simulated organic molecules that might be used for low cost, effective and easily produced materials to conduct and store solar energy. Harvard will work with Wolfram to make the seven million molecules and associated data publicly available by the end of 2012. This effort will provide valuable information to the materials community as it works to collectively to advance the MGI.

31 Companies and Academic Institutions Make Commitments to the MGI

31 organizations that represent a broad cross-section of the materials and manufacturing community have signed on to the <u>Orlando Materials Innovation Principles</u>, released by The Minerals, Metals & Materials Society (TMS). Signatories have pledged to advance the MGI vision by collaborating as a community, utilizing and developing new IT tools, and driving open models for data and knowledge sharing.

33 Universities Pledge to Train Materials Workforce of the Future

Led by the University Materials Council (UMC), 33 universities have pledged to pursue innovative new methods to train future materials scientists and engineers in ways that are consistent with the MGI vision. Areas of potential innovation are in new courses, use of computation tools in the classroom and new degree programs.

ASM International Launching Center to Accelerate Materials Data Exchange

A new Center for Computational Materials Science and Engineering Data will work to define protocols collecting, disseminating, and managing materials data. These protocols will enable the development of data "ecosystems" for sector-specific materials, such as aerospace, to develop, share, and manage large amounts of data.

Autodesk Releasing Library of 8000+ Materials and Resources to Educate Materials Workforce

Autodesk is making new simulation technology and a library of properties for more than 8000 materials available via the cloud to their more than 100,000 design customers. This technology was developed in cooperation with the Pacific Northwest National Laboratory, the University of Illinois at Urbana-Champaign and the Oak Ridge National Laboratory. Autodesk is also committed to making this new materials information available to the US educational community for use in the classroom which complements their recent release of Autodesk <u>Simulation</u> <u>Workshop</u>, a free online source of education modules that can be used to train the next generation of engineers in advanced materials use.

Lockheed Martin Leading New Carbon Nanostructures Consortium

Lockheed Martin has announced plans to establish an industry-led, multi-sector Carbon Nanostructures Consortium. The Consortium will work to accelerate the development and transition of affordable, high-performance carbon nanostructure-enhanced materials that have the potential to be transformative for energy, aerospace, and electronics.

General Electric (GE) Enhancing Industry-University-Public Interactions

In July of this year, GE Global Research will convene a Summit on Additive Manufacturing, bringing together design, material and process modeling technologies with manufacturing process development to drive faster adoption of this critical technology. This precedes a Lecture and Workshop series specifically devoted to the Materials Genome launching later this year. These steps to convene the community are complemented by an existing program where GE sponsors post-doctoral experts in the field on the topics of the MGI.

Together, the above commitments will support the MGI vision in three ways:

- By fostering a new "materials innovation infrastructure" in computation, experimentation, digital data and collaborative networks;
- By addressing high priority material problems of national importance; and
- By building a community that emphasizes workforce training and embraces a more collaborative approach to developing advanced materials.

BUILDING ON PROGRESS: BROAD ACTIVITIES BY NATIONAL LABS AND FEDERAL AGENCIES IN SUPPORT OF MGI

National Labs Joining Forces to Launch New Joint Materials Genome Institute

Responding to the challenge of the Materials Genome Initiative, Oak Ridge, Argonne and Lawrence Berkeley National Labs have come together to form a Joint Materials Genome Institute (JMGI) for accelerated discovery and design of advanced materials. The central element of JMGI is the development of new computational methods to predict the properties of materials, from catalysts and photovoltaics to lightweight structural materials. A broad-based design effort will apply these codes, taking into account the requirements of individual applications, to drive the choice of material composition, structure, synthetic pathways, and advanced manufacturing. The necessary verification of these design codes will be accomplished using state-of-the-art instrumentation. Finally, benchmark experimental results and data on materials properties will be archived in an environment that allows them to be exchanged among researchers and integrated into the design process. JMGI will also develop new teaching programs to train the next generation of researchers.

Argonne National Lab Assembling MGI Ecosystem in the Chicago Metropolitan Area

The U.S. Department of Energy's (DOE) Argonne National Laboratory is collaborating with Northwestern University, the University of Chicago and private sector – building new crossdisciplinary teams with increased access to Argonne's cutting-edge scientific tools, including Mira, a new 10-petaflop supercomputer. The expansion of the joint Northwestern-Argonne Institute will unite the laboratory's supercomputing capabilities with Northwestern's world-class materials research faculty and leverage the university's strong ties with the advanced materials industry. Argonne is working with the newly established Institute for Molecular Engineering at the University of Chicago to expand the region's capabilities in nanoscale technologies and materials design.

Berkeley National Lab Tripling Supercomputing Hours for Materials Project

Berkeley National Lab's National Energy Research Scientific Computing Center will triple supercomputing hours for the already successful <u>Materials Project</u> to 40 million hours by 2013. New plans are also underway to expand its supercomputing framework for material domains in carbon capture, advanced metal alloys, and critical materials.

National Nanotechnology Initiative Contributing to the MGI

The National Nanotechnology Initiative is launching a new signature initiative that advances the goals of the MGI. The Nanotechnology Knowledge Infrastructure (NKI) developed by ten federal agencies will stimulate the development of models, simulation tools, and databases that enable the prediction of specific properties and characteristics of nanoscale materials. Also, approaches, protocols, and standards developed through MGI activities may be initially explored, tested, or evaluated specifically for nanoscale materials under NKI efforts. This cross-fertilization between the NNI and MGI will yield broader knowledge dissemination and can be facilitated by the proposed NKI effort. [GET LINK FROM TOF]

DOE Leads MGI Efforts Across Multiple Programs

In FY2012, DOE is evaluating proposals for up to <u>\$12 million of research</u> in predictive theory and modeling for materials and chemical sciences. This research will combine computational tools, experimental tools, and digital data to advance materials and chemical processes; provide user friendly software that captures the essential physics and chemistry of relevant systems; and harness the power of modern experimental techniques. In a complementary effort, the DOE Office of Science is forming SciDAC (Scientific Discovery through Advanced Computing) partnerships between materials and chemical researchers, applied mathematicians, and computer scientists to exploit the most powerful computers available to develop new algorithms and computational approaches that could dramatically accelerate the discovery of new materials and processes critical to the MGI. DOE's Office of Science also provides funding for the Computational Materials and Chemical Sciences Network of inter-disciplinary teams that develop and test new software of relevance to materials and chemical processes. DOE's Office of Energy Efficiency and Renewable Energy continues to integrate MGI principles throughout its various energy technology research activities, including a \$14M light-weighting effort in the Vehicle Technologies Program and the Hydrogen and Fuel Cells Technologies Program. The Hydrogen Fuel Cell Technology Program alone has allowed millions of unique material compositions to be screened computationally, and hundreds of materials to be investigated experimentally.

NIST Leads Measurements & Standards Efforts to Support MGI

NIST is actively engaged with stakeholders from industry, academia and government to develop: (1) standards and tools for the representation and interoperability of materials data, whether from simulation or experiment, (2) techniques and standards for the interoperation of modeling systems operating at multiple length and time scales and techniques, and (3) tools for the quality

assessment of models, simulations, and the materials data generated from them. These techniques, standards, and tools will provide materials property data and related software to the research community. The NIST Advanced Materials for Industry program will also support a series of workshops to identify and develop the measurements and standards necessary for the MGI.

NSF Funds Transformative Approaches that Support MGI

NSF has launched its Designing Materials to Revolutionize and Engineer our Future (DMREF) program in support of the MGI. The program is spearheaded jointly by NSF's Mathematical and Physical Sciences (MPS) and Engineering (ENG) Directorates to fund transformative approaches to accelerate materials discovery, development and manufacturing, and to advance fundamental materials understanding so that material properties can be predicted, optimized, and ultimately controlled through design. NSF will make the first DMREF awards this summer and intends to continue the program in upcoming years. Other related NSF initiatives include Cyber-infrastructure for the 21st Century, CIF21, and Core Techniques and Technologies for Advancing Big Data Science & Engineering.

DOD Invests in Research for Materials Innovation Infrastructure

The DOD is investing \$17.3 million in 2012 to extend basic research in support of the MGI. The Office of Naval Research has awarded basic research projects that integrate analysis with materials research to improve the prediction and optimization of materials properties through new approaches to modeling material characteristics. The Army Research Laboratory recently announced the launch of two basic research collaborative enterprises to create the scientific basis to design materials suitable for the unique requirements of the Nation's Soldiers. A consortium led by Johns Hopkins University will develop new materials that have been predictably and reliably designed to protect Soldiers in extreme dynamic environments. The University of Utah will lead a team to further the capability to develop sophisticated electronic materials through multidisciplinary and multi-scale modeling. The Air Force Research Laboratory (AFRL) will be awarding a university center of excellence focused on developing the fundamental science of computational and experimental methods common to all structural materials. AFRL also announced it will award efforts to solve two foundational engineering problems in the areas of nickel-based superalloys for jet engines and organic matrix composites for aerospace structures. These efforts will demonstrate the reduced cost and development time that can be delivered through the MGI paradigm.

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