Research Activity: **Atomic, Molecular, and Optical Science**
Division: Chemical Sciences, Geosciences, and Biosciences
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Portfolio Description:

The Atomic, Molecular, and Optical Science (AMOS) activity supports basic research on fundamental interactions among atoms, molecules, electrons, and photons. The program supports experiments and theory to understand and control ultrafast interactions of intense electromagnetic fields with atoms and molecules, correlated many-body interactions in systems far from equilibrium, novel chemical and emergent phenomena in ultracold ensembles of atoms and molecules, and light-matter interactions on the nanometer length scale and sub-picosecond time scale. The activity strongly supports development and application of novel x-ray light sources and ultrafast probes to enable future research in the chemical sciences and to enable research at current and planned BES user facilities. By studying the fundamental interactions among atoms and molecules, AMOS provides the foundation for understanding chemical reactivity, i.e., the process of energy transfer between molecules and ultimately the making and breaking of chemical bonds.

Unique Aspects:

The knowledge and techniques developed in the AMOS activity broadly enable the fundamental science efforts of the Department of Energy (DOE), including research conducted at BES user facilities. The results of this research have wide applicability in enabling science and technology. The AMOS activity provides new ways to control and probe interactions in the gas and condensed phases, enhances our ability to understand materials of all kinds, and enables full exploitation of the BES x-ray sources and Nanoscale Science Research Centers (NSRCs). This enabling aspect will continue to be emphasized, particularly with respect to research into the generation and application of ultrashort, intense x-ray pulses. The AMOS activity includes ultrashort x-ray pulse generation and applications at the Advanced Light Source (ALS), the Advanced Photon Source (APS), the Photon Ultrafast Laser Science and Engineering (PULSE) Center, and the Ultrafast X-ray Science Laboratory (UXSL). AMOS is a major supporter of synchrotron-based AMO science in the United States, and continues its role as the principal U.S. supporter of research into the properties and interactions of atomic and molecular ions relevant to fusion plasmas.

Relationship to Other Programs:

The AMOS program supports planned experiments concerning x-ray characterization and AMO science at the Linac Coherent Light Source (LCLS) at the Stanford Linear Accelerator Center (SLAC), in coordination with the BES Scientific User Facilities Division. The AMOS program funds research at the new PULSE center at SLAC, which is co-supported by the BES Materials Sciences and Engineering Division, and the UXSL at Lawrence Berkeley National Laboratory (LBNL). Numerous complementary relationships exist between AMOS program elements and other core research activities across the BES Chemical Sciences, Geosciences, and Biosciences Division. Fundamental insight and data obtained in the AMOS activity are relevant to Office of Fusion Energy Sciences (FES) programs in atomic data for fusion modeling and basic plasma physics. This synergy is notable at the Multicharged Ion Research Facility (MIRF) at Oak Ridge National Laboratory (ORNL), which is co-funded by BES and FES. A close working relationship exists with the National Science Foundation (NSF) Atomic, Molecular, Optical and Plasma Physics Program. These two programs co-funded the National Academy of Sciences/National Research Center Physics Decadal Survey, *"AMO 2010: An Assessment of and Outlook for Atomic, Molecular, and Optical Science."* In FY 2007, the AMOS Program provided partial support for the Gordon conferences on Quantum Control of Light and Matter, and Atomic Physics, the conference on Fundamental Optical Processes in Semiconductors, and the Joint Conferences on Ultrafast Optics and Applications of High Field and Short Wavelength Sources. In FY 2008, the AMOS program provided partial support for the Gordon conference on Photoions, Photoionization and Photodetachment.

Significant Accomplishments:

The AMOS activity has been a major U.S. supporter of experimental and theoretical studies of the fundamental properties of atoms, ions, and small molecules and of collisional interactions between atoms, ions, molecules, and surfaces. This has produced a vast knowledge base, with a broad impact on science and technology. It has led to the development of powerful new methods for momentum imaging of collision fragments that have seen wide application in atomic, molecular, and chemical physics. This knowledge is now being used to manipulate the quantum behavior of atoms and molecules and has propelled further development and scientific applications of ultrafast x-ray sources using table-top lasers and 3rd generation synchrotrons (ALS and APS). Enhanced high-harmonic generation and fundamental interactions of intense controlled laser fields with atoms and small molecules leading to ionization and fragmentation have been explored. Recent efforts involving high-field interactions, ultrafast processes, and ultrashort x-ray pulses are creating the science base required for research at 4th generation light sources such as the LCLS. X-ray pulses with durations of femtoseconds can produce stop-action pictures of the motion of atoms during molecular transformations. New sources, with pulses of attosecond duration may make it possible to image the real-time motion of the electrons during the course of chemical reactions. Recent progress has been reported in the generation of ultrashort x-ray pulses from table-top, laser-based sources that provide complementary capabilities to planned x-ray free electron lasers, such as the LCLS. In one example, hard-x-ray pulses were generated from a liquid mercury target irradiated by high power, femtosecond laser pulses. In another approach, high harmonic generation in gases has been used to shift laser light from the infrared or visible to extreme-ultraviolet or soft x-ray wavelengths. Suitable optical manipulation of the harmonics can be used to produce x-ray pulses of a few attoseconds in duration. Finally, theorists have suggested a method to use intense, ultrafast laser pulses to make a gas transparent to x-rays for the duration of the laser pulse. If realized experimentally, this device could be used as an ultrafast switch to slice a femtosecond pulse from a much longer x-ray pulse. Recognition of international scientific leadership by AMOS-sponsored investigators includes MacArthur, Rabi, Goeppert-Mayer, Davisson-Germer awards; American Physical Society Fellowships; and National Academy memberships.

Mission Relevance:

AMO science empowers a wide spectrum of DOE research activities and lays the scientific foundation for research performed at BES scientific facilities. New ways to control and probe interactions in the gas and condensed phases enhance our ability to understand materials of all kinds and enable the full exploitation of the BES x-ray sources and NSRCs. The study of intense field and ultrafast x-ray interactions provides a basis of understanding essential for experiments anticipated at 4th generation light sources. The research on many-body phenomena addresses issues of chemical reactivity important to DOE, such as electron-driven processes relevant to radiation chemistry and reactions of ions and other species important to fusion plasmas. Research on ultracold atoms and molecules explores regimes of behavior and control that are inaccessible under normal conditions, enabling careful manipulation and investigation of long-range cooperative effects, complex interactions, and emergent phenomena. The effort to understand nanoscale light-matter interactions is central to research in photo-energy conversion relevant to the use of solar energy, enables the development of scientific tools for nanoscale materials characterization and chemical imaging, and advances our ability to study and control the properties of matter and chemical reactivity on the nanometer length scale and sub-picosecond time scale. AMOS contributes at the most fundamental level to the science-based optimization of current energy sources and the development of new sources.

Scientific Challenges:

In recent years, AMO science has seen a transformation; it has changed from a field in which the fundamental interactions of atoms, molecules, photons, and electrons are probed to one in which they are controlled. Systems studied are increasingly complex. Correlated, non-perturbative interactions are the norm. AMOS practitioners can now shape the quantum mechanical wave functions of atoms and small molecules using controllable laser fields; trap and cool atoms and molecules to temperatures near absolute zero where cooperative phenomena can be precisely controlled; create nanoscale structures that manifest novel light-matter interactions and properties; and coherently drive electrons in atoms, plasmas, or synchrotron orbits to generate ultrafast x-ray pulses. Theoretical advances are enabling modeling and simulation of increasingly complex systems to provide interpretation of existing data and predictions for new experiments. These capabilities create opportunities to investigate chemical processes under conditions that are far from equilibrium, where complex phenomena are predominant and controllable, and on ultrafast timescales commensurate with the motions of atoms and electrons. Research in AMO science is fundamental to meeting the grand challenges for basic energy sciences, as identified in the recent report on this topic from the Basic Energy Sciences Advisory Committee.

Funding Summary:

Dollars in Thousands

FY 2007	FY 2008	FY 2009 Request
18,112	18,112	23,659

Performer	Funding Percentage
DOE Laboratories	48 %
Universities	52 %

These are percentages of the operating research expenditures in this area; they do not contain laboratory capital equipment, infrastructure, or other non-operating components.

The AMOS activity provides funding for 53 university grants that partially support about 60 faculty and senior staff. It also funds 4 programs at national laboratories, supporting about 20 senior staff. Programs at the laboratories are multi-investigator efforts focusing on problems that require extensive participation by senior scientists and postdoctoral associates. These programs capitalize upon unique facilities at the DOE national laboratories, including the MIRF at ORNL, the ALS at LBNL, the APS at Argonne National Laboratory (ANL), and the LCLS which will be operational in 2009 at SLAC. A program at Los Alamos National Laboratory (LANL) on optical properties of semiconductor nanocrystals is strongly affiliated with the new Center for Integrated Nanotechnologies at LANL and Sandia National Laboratories (SNL). The activity also supports the J. R. MacDonald Laboratory at Kansas State University, a multi-investigator program devoted to the experimental and theoretical study of intense-field physics produced by ultrafast lasers or collisions with highly charged ions.

Projected Evolution:

The AMOS activity will continue to support AMO science that advances DOE and BES mission priorities. Closely related experimental and theoretical efforts will be encouraged. AMOS will continue to have a prominent role in at BES facilities in understanding the interaction of intense, ultrashort x-ray pulses with matter; in the control and investigation of light-matter interactions with nanoscale structures; and in the investigation of ultrafast processes. Key targets for greater investment include: ultrafast electron diffraction; attosecond physics with phase-controlled pulses; electron-driven processes; quantum control of molecular processes; and nonlinear optics relevant to ultrafast, short wavelength, and nanoscale physics.

The program will strongly emphasize ultra-fast, ultra-intense, and short-wavelength science. The development and application of novel x-ray light sources using existing synchrotrons or table-top lasers will continue. Topics of interest include the development of high-harmonic generation or its variants as soft x-ray sources, development and characterization of femtosecond and attosecond pulses of x-rays at existing synchrotrons as well as new accelerator-based and table-top sources, and applications in the chemical and materials sciences. Coherent control of nonlinear optical processes and tailoring quantum mechanical wavefunctions with lasers will grow in importance, particularly in chemical systems.

Opportunities include theory and experiment for artificial nano structures in materials and their interactions with light, and the use of nonlinear spectroscopies to characterize the optical properties of nanoscale systems. Studies of the creation of ultracold ensembles of atoms and molecules to investigate and control long range cooperative or emergent phenomena and chemical interactions under these conditions will continue. Fundamental studies of atomic and molecular ions and their interactions with atoms, molecules, and surfaces will further develop the knowledge base vital to understanding fusion plasmas. Experimental and theoretical AMOS tools will be used in the study of low-energy electron-molecule interactions in the gas and condensed phases.