Research Activity: Atomic, Molecular, and Optical Sciences

Division: Chemical Sciences, Geosciences, and Biosciences
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Portfolio Description:

The Atomic, Molecular, and Optical Sciences (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 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 underpin other fundamental science efforts of the Department of Energy (DOE), including research conducted at BES user facilities, as well as having wide applicability in enabling science and technology. The AMOS activity provides new ways to control and probe interactions in the gas and condensed phases, enhancing our ability to understand materials of all kinds and enabling 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) and Advanced Photon Source (APS), and it is the major supporter of synchrotron-based AMO science in the United States. The AMOS program continues its role as the principal U.S. supporter of research into the properties and interactions of highly charged atomic ions, which is of direct consequence to fusion plasmas.

Relationship to Other Programs:

The AMOS program supports current and planned experiments concerning x-ray characterization and AMO science at the Sub-Picosecond Photon Source (SPPS) and 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 Ultrafast Science Center at SLAC which is supported by the BES Materials Sciences and Engineering Division. The AMOS activity co-funds with the BES Condensed Matter Physics activity an ultrafast x-ray beamline at the ALS. 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. The AMOS program also elucidates interactions of intense laser fields with high-energy plasmas which are relevant to defense programs in DOE. A close working relationship exists with the National Science Foundation (NSF) Atomic, Molecular, Optical and Plasma Physics Program, and these two program are co-funding 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 2005, the AMOS Program provided partial support for the 10th International Conference on Multiphoton Processes (ICOMP2005) and the 2005 Gordon Conference on Atomic Physics.

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 on the properties of atoms, ions, and small molecules, 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. The 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 (HHG) using quasiphase matching and ionized atoms for soft x-ray production has been demonstrated, 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 the research that will be done at 4th generation light sources like the LCLS. Highlights from the past year include: detailed measurements and exact computations to understand the molecular breakup triggered by absorption of hard x-ray photons, such as will be prevalent with 4th-generation x-ray sources; observation of carrier multiplication in nanocrystals by which single photons produce multiple charge carriers, possibly providing a path toward more efficient solar energy conversion; observation of superfluidity in an ultracold Fermi gas of atoms, which may provide insight into other strongly interacting systems of particles such as the electrons in high T_C superconductors; and recognition of international scientific leadership by AMOS-sponsored investigators through MacArthur, Rabi, Goeppert-Mayer, Davisson-Germer awards, American Physical Society Fellowships, and National Academy memberships.

Mission Relevance:

AMO science underpins 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 including 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 research to understand nanoscale light-matter interactions underpins research in photo-energy conversion relevant to the use of solar energy, enables the development 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 scale. Thus AMOS contributes at the most fundamental level to the science-based optimization of current energy sources and the development of new ones.

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 wavefunctions 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 which manifest novel light-matter interactions and properties; and coherently drive electrons in atoms, plasmas, or synchrotron orbits to generate ultrafast x-ray pulses. These capabilities create opportunities to investigate chemical processes under conditions which are far from equilibrium, where complex phenomena are predominant and controllable, and on ultrafast timescales commensurate with the motions of atoms and electrons.

Funding Summary:

Dollars in Thousands

FY 2005	FY 2006	FY 2007 Request
16,627	15,397	19,248

Performer	Funding Percentage
DOE Laboratories	39 %
Universities	60 %
Other	1 %

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 activity provides funding for 55 university grants partially supporting 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 underscore unique facilities at the DOE national laboratories, including the MIRF at ORNL, the ALS at Lawrence Berkeley National Laboratory (LBNL), and the APS at Argonne National Laboratory (ANL). 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 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 either by ultrafast lasers or collisions with highly charged ions.

Projected Evolution:

The AMOS activity will continue support for 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 for molecular processes; ultracold molecular interactions, 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 pulses of x-rays at existing synchrotrons and new accelerator-based 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. Opportunities also include 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.
Fundamental studies of highly charged ions and their interactions with atoms, molecules, and surfaces will continue to further develop the knowledge base important to fusion plasmas. Opportunities include the use of the experimental and theoretical AMOS tools in the study of low-energy electron-molecule interactions in the gas and condensed phases.