Atomic, Molecular, and Optical Sciences

Portfolio Description

This activity supports theory and experiments to understand structural and dynamical properties of atoms, molecules, and nanostructures. The research emphasizes the fundamental interactions of these systems with photons and electrons to characterize and control their behavior. These efforts aim to develop accurate quantum mechanical descriptions of properties and dynamical processes of atoms, molecules, and nanoscale matter. The study of energy transfer within isolated molecules provides the foundation for understanding chemical reactivity, i.e., the process of energy transfer to ultimately make and break chemical bonds. Topics include the development and application of novel, ultrafast optical probes of matter, particularly x-ray sources; the interactions of atoms and molecules with intense electromagnetic fields; and studies of collisions and many-body cooperative interactions of atomic and molecular systems, including ultracold atomic and molecular gases. Capital equipment funding is provided for items such as lasers and optical equipment, unique ion sources or traps, position-sensitive and solid-state detectors, control and data processing electronics, and computational resources.

Unique Aspects

The knowledge and techniques developed by investigators in the AMOS program are critical components of the fundamental science effort of the Department of Energy (DOE), and research conducted at BES user facilities. The results of this research have applicability in a wide array of 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, 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 involving the generation and application of ultrafast, intense x-ray pulses at Lawrence Berkeley National Laboratory (LBNL) at the Advanced Light Source (ALS) and the Ultrafast X-ray Science Laboratory (UXSL); at Argonne National Laboratory (ANL) at the Advanced Photon Source (APS); and at SLAC National Accelerator Laboratory (SLAC) at the Linac Coherent Light Source (LCLS) and the PULSE Institute for Ultrafast Energy Science (PULSE). 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 experiments concerning x-ray characterization and AMO science at the LCLS at SLAC, in coordination with the BES Scientific User Facilities Division. The program funds research at the PULSE Institute for Ultrafast Energy Science at SLAC, which is co-supported by the BES Materials Sciences and Engineering Division. 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 to provide atomic and molecular 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 and Optical 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, and co-fund the National Academy of Sciences Committee on Atomic, Molecular, and Optical Sciences (CAMOS). In FY 2008, the AMOS Program provided partial support for the Gordon conference on Multiphoton Processes and the American Conference on Theoretical Chemistry (ACTC). In 2009, the Program provided partial support for the Attosecond Physics meeting at Kansas State University, and the Materials Research Society (MRS) Symposium on Ultrafast Materials Sciences.

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 collision 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 being used to control 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 in great detail. 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 enable imaging of the real-time motion of 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 x-ray free electron lasers. In one example, 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. Optical manipulation of the harmonics has been used to produce isolated XUV (extreme ultraviolet) pulses as short as 100 attoseconds in duration. Theorists suggested a method to use intense, ultrafast laser pulses to make a gas transparent to x-rays for the duration of the laser pulse. This prediction has been verified in experiments at the ultrafast slicing source at the ALS. This method may find application 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 include MacArthur, Rabi, Goeppert-Mayer, Davisson-Germer awards, American Physical Society Fellowships, and National Academy memberships.

Mission Relevance

The knowledge and techniques produced by this activity form a science base that underpins several aspects of the DOE mission. New methods for using photons, electrons, and ions to probe matter lead to more effective use of BES synchrotron, nanoscience, and microcharacterization facilities. Similarly, the study of formation and evolution of energized states in atoms, molecules, and nanostructures provides a fundamental basis for understanding elementary processes in solar energy conversion and radiation-induced chemistry.

Scientific Challenges

In recent years, AMO science has transformed 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, and exhibit highly correlated, non-perturbative interactions. AMOS scientists can 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, create nanoscale structures that manifest novel light-matter interactions and properties, and coherently drive electrons 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 report from the Basic Energy Sciences Advisory Committee: *Directing Matter and Energy: Five Challenges for Science and the Imagination.*

Projected Evolution

The AMOS activity will continue to support 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 at BES facilities in understanding the interaction of intense, ultrashort x-ray pulses with matter and in the control and investigation of ultrafast light-matter interactions. Key targets for greater investment include: ultrafast electron diffraction; attosecond physics with phase-controlled pulses; electron-driven processes; quantum control of molecular processes; nonlinear optics relevant to generating ultrafast, short wavelength pulses; and nanoscale physics.

The program will emphasize ultrafast, ultra-intense, short-wavelength science. The development and application of novel x-ray light sources using synchrotrons or table-top lasers will continue. Topics of interest include the use 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. Applications of these light sources include ultrafast imaging of chemical reactions, diffraction from aligned molecules, and atomic and molecular inner-shell photoionization. Coherent control of nonlinear optical processes and tailoring quantum mechanical wave functions with lasers will continue, particularly in chemical systems. 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, and collisions of ultracold molecules.