Atomic, Molecular, and Optical Sciences

Portfolio Description

This activity supports theory and experiments to understand structural and dynamical properties of atoms, molecules, and nanostructures. 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. The study of energy transfer within isolated molecules provides the foundation for understanding chemical reactivity, the processes of energy transfer that make and break chemical bonds. Topics include the development and application of novel, ultrafast optical probes of matter, particularly with x-rays; the interactions of atoms and molecules with intense electromagnetic fields; and studies of collisions and many-body cooperative interactions of atomic and molecular systems. Capital equipment funding is provided for items such as lasers and optical components, 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 Atomic, Molecular, and Optical Sciences (AMOS) program are critical components of the fundamental science effort of the Department of Energy (DOE), and research conducted at Basic Energy Sciences (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.

Relationship to Other Programs

- The program supports experiments involving 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.
- A close working relationship exists with the National Science Foundation (NSF) Atomic Molecular and Optical Physics Programs. These programs co-fund studies by the National Academies in relevant areas and the National Academies' Committee on Atomic, Molecular, and Optical Sciences (CAMOS).

Significant Accomplishments

The AMOS activity has been a major 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 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 third 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 fourth 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 accomplishments in the program include:

- Generation of ultrashort x-ray pulses from table-top, laser-based sources to provide complementary capabilities to x-ray free electron lasers.
- High harmonic generation in gases has been used to shift laser light from the infrared or visible to extreme-ultraviolet and soft x-ray wavelengths.
- Optical manipulation of the harmonics has been used to produce isolated extreme ultraviolet pulses shorter than 100 attoseconds in duration.
- AMOS scientists were deeply involved in commissioning and early experiments at the LCLS. Results at this facility include inner-shell photoionization of atom and molecules, single-particle imaging of nanoparticles, inner-shell lasing, and non-linear x-ray spectroscopy.

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, free-electron laser, and nanoscience facilities. Similarly, studies of formation and evolution of highly-excited states of atoms, molecules, and nanostructures provide 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, 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 scientists will continue to have a prominent role at BES user 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 complex chemical systems. Experimental and theoretical AMOS tools will be used in the study of low-energy electron-molecule interactions in the gas and condensed phases.