Atomic, Molecular, and Optical Sciences

Portfolio Description

This program supports basic experimental and theoretical research aimed at understanding the structural and dynamical properties of atomic and molecular systems. The research focuses on fundamental interactions of these systems with photons and electrons to characterize and control their behavior. The goal is to develop accurate quantum-mechanical descriptions of dynamical processes such as chemical bond breaking and forming, interactions in strong fields, and electron correlation. Topics of interest include the development and application of novel, ultrafast probes of matter; the interactions of atoms and molecules with intense electromagnetic fields; and quantum control of atomic and molecular systems.

Scientific Challenges

In recent years, atomic, molecular, and optical science (AMOS) 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. 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 drive electrons coherently 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 AMOS is fundamental to meeting the grand challenges for basic energy sciences, as identified in the 2007 report from the Basic Energy Sciences Advisory Committee, *Directing Matter and Energy: Five Challenges for Science and the Imagination*, and reiterated in the 2015 report, *Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science* (https://science.energy.gov/bes/community-resources/reports/).

Projected Evolution

The program emphasizes ultrafast, strong-field, short-wavelength science, and correlated dynamics in atoms and molecules. The AMOS program will continue to have a prominent role at Basic Energy Sciences (BES) facilities in understanding and controlling the interaction of intense, ultrafast extreme ultraviolet and x-ray pulses with matter. Examples include the use of high-harmonic generation or its variants as soft x-ray sources; intense, ultrafast x-ray science at the Linac Coherent Light Source (LCLS); and development and characterization of femtosecond and attosecond pulses of x-rays at accelerator-based and table-top sources. Applications at these light sources include ultrafast imaging of chemical reactions, diffraction and harmonic generation from aligned molecules, and inner-shell photoionization of atoms and molecules. Coherent control of nonlinear optical processes and tailoring of quantum-mechanical wave functions with lasers will continue to be of interest, particularly in molecular systems. Experimental and theoretical tools will be used to study low-energy electron-molecule interactions in the gas and condensed phases. Key targets for greater investment include attosecond science, ultrafast x-ray science, and ultrafast electron diffraction from molecular systems.

The AMOS program is not accepting applications in the areas of nanoscience, bioscience, and science of ultracold systems.

Significant Accomplishments

The AMOS program has been a major supporter of experimental and theoretical studies of the fundamental properties of atoms, ions, and small molecules and their interactions with photons and electrons. This activity 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 (i.e., the Advanced Light Source and the Advanced Photon Source). 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. Efforts involving high-field interactions, ultrafast processes, and ultrashort x-ray pulses continue to build the science foundation required for research at x-ray free-electron lasers 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, producing attosecond-duration pulses, 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 and solids has been used to shift laser light from the infrared or visible to extreme-ultraviolet and soft x-ray wavelengths.
- Optical manipulation of the harmonic-generation process has been used to produce isolated extreme ultraviolet pulses with linear or circular polarization and with pulse durations shorter than 100 attoseconds.
- New sources and methods have been developed to use ultrafast electron diffraction for three-dimensional imaging of gas-phase species, providing sub-angstrom spatial resolution and femtosecond time resolution.
- AMOS scientists were deeply involved in commissioning and early experiments at the LCLS and have continued to lead and contribute to many ground-breaking experiments. In addition to leading development of an x-ray split-and-delay instrument and the imaging end-station, AMOS researchers have led pioneering experiments to develop a fundamental, quantitative understanding of the complex molecular dynamics induced by very-high-intensity ultrafast x-ray pulses. Results at this facility also include single-particle imaging of nanoparticles, inner-shell lasing, and non-linear x-ray spectroscopy. AMOS scientists continue today to set the stage for new breakthroughs to exploit next-generation capabilities that will be available when the LCLS-II construction project is completed.
- Pump-probe techniques using ultrafast x-rays have enabled ultrafast chemical dynamics measurements with atomic specificity and femtosecond time resolution.

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 light sources. This enabling aspect will continue to be emphasized, particularly with respect to research involving the generation and application of ultrafast, intense x-ray and extreme ultraviolet light pulses using the Advanced Light Source at Lawrence Berkeley National Laboratory (LBNL), the Advanced Photon Source at Argonne National Laboratory, and the LCLS and the Stanford Synchrotron Radiation Lightsource at SLAC National Accelerator Laboratory (SLAC). This area of research benefits from research efforts in the Ultrafast X-ray Science Laboratory at LBNL and the PULSE Institute for Ultrafast Energy Science at SLAC. The AMOS program is a major supporter of synchrotron-based and x-ray free-electron-laser-based atomic, molecular, and optical science in the United States.

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 ultrafast electron diffraction 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.

Relationship to Other Programs

- The program supports experiments involving ultrafast x-ray characterization and AMOS at the LCLS at SLAC, in coordination with the BES Scientific User Facilities Division.
- Numerous complementary relationships exist between the AMOS program and other core research activities across the BES Chemical Sciences, Geosciences, and Biosciences Division in the development and application of ultrafast methods to elucidate and control molecular dynamics and charge transport important for photochemical reactions and light-harvesting applications.
- A close working relationship exists with the National Science Foundation (NSF) Atomic Molecular and Optical Physics program. AMOS and NSF have co-funded the National Academies' activities sponsored by the Committee on Atomic, Molecular, and Optical Sciences.