Research Activity: **Atomic, Molecular, and Optical Science**
Division: Chemical Sciences, Geosciences, and Biosciences
Primary Contact(s): Eric Rohlfing (eric.rohlfing@science.doe.gov ; 301-903-8165)
Team Leader: Eric Rohlfing
Division Director: Walter Stevens

Portfolio Description:

The AMOS activity supports experimental and theoretical studies of the fundamental properties of atoms, ions, and small molecules and the interactions between electrons, photons, and ions in collisions with atoms, molecules, and surfaces. Research is aimed at the most complete quantum mechanical description of such properties and interactions. Topics of interest include: studies of the interactions of intense electromagnetic fields, induced by highly charged ions or lasers, with atoms and molecules; coherent control of quantum mechanical processes; development and application of novel x-ray light sources in advance of next generation light sources; theory and experiment on ultracold collisions and quantum condensates.

Unique Aspects:

The underpinning aspect of the AMOS activity gives it a unique relationship with BES activities that utilize photon, electron, neutron, and heavy ion probes at the BES user facilities. The relationship will continue to be exploited, particularly with respect to forefront research into the generation and application of ultrashort, intense x-ray pulses. The AMOS program is the sole supporter of synchrotron-based AMOS studies in the U.S., which includes ultrashort x-ray pulse generation and utilization at the ALS and APS. 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. The program supports unique ion source/trap and accelerator facilities to conduct this work.

Relationship to Others:

The AMOS activity funds with BES Materials Science the ultrafast x-ray beamline at the ALS. The program has had substantial participation in the continued development of the scientific case for the Linac Coherent Light Source (LCLS), and several AMOS PIs serve on the LCLS Scientific Advisory Committee. Fundamental insight and data obtained in the AMOS activity are relevant to FES programs in atomic data for fusion modeling and basic plasma physics. This synergy is particularly noticeable at the Multicharged Ion Research Facility (MIRF) at ORNL, which is co-funded by BES and FES. There is overlap in the interactions of intense laser fields with high-energy plasmas relevant to defense programs in DOE. A close working relationship exists with the NSF Atomic, Molecular, Optical and Plasma Physics Program, and these two programs co-fund the NAS/NRC Committee on Atomic, Molecular and Optical Science (CAMOS). In 2002, the AMOS Program provided partial support for the Gordon Conference on Multiphoton Processes and the 8th International Conference on X-Ray Lasers. The program had active participation in the workshop at PNNL on Understanding the Role of Water in Electron-Initiated Processes and Radical Chemistry that involved both chemical physicists and radiation chemists supported by BES.

Significant Accomplishments:

During the past five years, 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 lead to the acquisition of a vast database on the properties of atoms, ions and small molecules. This information is now being used to manipulate the quantum behavior of these species. It has also lead to the development and application of powerful new methods for momentum imaging of collision fragments that have seen wide application in atomic, molecular, and chemical physics. More recently, the initiative on Novel X-Ray Light Sources has lead to the further development and scientific application of ultrafast x-ray sources using table-top lasers and 3rd generation synchrotrons (ALS and APS). Quasi phase matching of high-harmonic generation for soft x-ray production has been demonstrated and fundamental interactions of intense and controllable laser fields with atoms and small molecules leading to ionization and fragmentation have been examined. New projects in FY2002 focused on electron-driven processes in gaseous and condensed phases, the production and utilization of ultracold molecules and multidimensional spectroscopy for characterization of the optical properties of nanoscale materials. Prof. John Thomas of Duke University observed a possible superfluid transition in an ultracold Fermi gas, an observation with important ramifications for our fundamental understanding of cooperative phenomena in Fermionic systems. Prof. Philip Bucksbaum at the University of Michigan took the first steps toward creation of an ultrafast x-ray switch in work done on laser-modulated x-ray diffraction at the Advanced Photon Source. Dr. Fred Meyer at ORNL performed benchmark studies of how highly charged ions are neutralized in collisions with metal surfaces using the MIRF at ORNL. Dr. Debbie Jin of JILA/University of Colorado was awarded the 2002 Maria Goeppert-Mayer Award by the American Physical Society for her pioneering work on quantum degenerate Fermi gases. In 2002 four AMOS PIs were named Fellows of the American Physical Society; 68% of the current PIs in the program are now Fellows.

Mission Relevance:

AMO Science underpins a wide spectrum of BES research activities and lays the foundation for enhanced future utilization of BES light sources, electron beam microcharacterization centers, and neutron scattering facilities. The knowledge and techniques acquired through the AMOS program have potential impact in the development of new probes of matter in the gas and condensed phases using photons, electrons, and ions; on our understanding of nanostructured materials; and on our ability to model low- and high-temperature plasmas. AMOS contributes at the most fundamental level to the science-based optimization of current energy sources and the development of new ones.

Scientific Challenges:

AMO science is currently undergoing a transition from a field in which the fundamental interactions of atoms and molecules are probed to one in which they are *controlled*. The enormous database of knowledge acquired over the last several decades and the powerful technical innovations in laser technology are the two forces driving this transition. AMOS practitioners can now shape the quantum mechanical wavefunctions of atoms and small molecules using controllable laser fields, trap and cool atoms (and soon molecules) to temperatures near absolute zero where condensation into a single quantum state occurs, create coherent matter waves by manipulating quantum condensates, create novel surface structures using highly charged ion beams, and coherently drive electrons in atoms so that they generate high-harmonic radiation in the soft x-ray region.

Funding Summary:

Dollars in Thousands

FY 2002	FY 2003 Request	FY 2004 Request
11,815	11,815	12,275

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Performer	Funding Percentage
DOE Laboratories	39.0%
Universities	60.0%
Other	1.0%

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 program provides funding for 47 university grants supporting about 60 students and partially supporting about 55 faculty and senior staff. It also funds 3 programs at national laboratories supporting about 15 senior staff and 3 students and postdocs. Programs at the laboratories are multi-investigator efforts focusing on problems that require extensive participation by experienced scientists. These programs usually underscore the user facilities at the SC laboratories, including the Multicharged Ion Research Facility (MIRF) at ORNL, the ALS at LBNL and the APS at ANL. A new program at LANL on optical properties of semiconductor quantum dots, which was funded under NSET in FY2002, is strongly affiliated with the nascent Center for Integrated Nanotechnologies at LANL/SNL. The program supports the J. R. MacDonald Laboratory at Kansas State University: a multi-investigator program and BES Collaborative Research Center devoted to the experimental and theoretical study of collisional processes involving highly charged ions.

Projected Evolution:

Coherent control of nonlinear optical processes and tailoring quantum mechanical wavefunctions with lasers will grow in importance. Such control will be vital to the ultimate realization of laser-controlled chemistry and to our ability to store and read information in quantum systems.

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 useable soft x-ray sources, development and characterization of femtosecond pulses of x-rays at existing synchrotrons and applications in the chemical and materials sciences.

AMO science plays a strong role in nanoscale science efforts. Opportunities include the development of AMO theory for artificial quantum structures in materials, the utilization of light force trapping and cooling to create ultracold samples of atoms and molecules including quantum condensates, the use of nonlinear spectroscopies to characterize the optical properties of nanoscale materials and the manipulation of condensates to create coherent matter waves. Quantum condensates of bosons and fermions represent novel nanostructures whose properties (superfluidity, Cooper pairing, etc.) increasingly blur the boundary between atomic and condensed matter physics. Coherent matter waves offer dramatic opportunities for atom lithography on the nanoscale.

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. A new thrust area related to this effort will be to utilize the experimental and theoretical tools of AMOS in the study of low-energy electron-molecule interactions in the gas and condensed phases. Such interactions play vital roles in determining the subsequent chemistry in low-temperature plasma processing, which is used extensively in the semiconductor industry and in radiation environments such as mixed-waste storage tanks.

April 7, 2003