Research Activity: Atomic, Molecular, and Optical Science

Division: Chemical Sciences, Geosciences, and Biosciences

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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: 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 a major supporter of synchrotron-based AMOS studies in the U.S., which includes ultrashort x-ray pulse science and high-resolution spectroscopy 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.

Relationship to Others:

The AMOS activity co-funds with BES Condensed Matter Physics an ultrafast x-ray beamline at the ALS. The program has contributed substantially to ongoing and planned experiments concerning x-ray characterization and AMO science at the Sub-Picosecond Photon Source (SPPS) and Linac Coherent Light Source (LCLS) at SLAC. Fundamental insight and data obtained in the AMOS activity are relevant to Fusion Energy Science 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 FY2003, the AMOS Program provided partial support for three Gordon Conferences: Quantum Control of Light and Matter; Photoions, Photoionization and Photodetachment; and Atomic Physics. The program had active participation in the Conference on Super Intense Laser Atom Physics (SILAP) that involved an international community of scientists who are interested in the interaction of intense laser fields with matter.

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 (HHG) 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 2003 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. Some of the program's highlighted work and awards from the year include: Professors Margaret Murnane and Henry Kapteyn and co-workers at the University of Colorado used a waveguide to limit plasma-induced defocusing and generate HHG in argon at photon energies up to 250 eV, significantly extending its range. Dr. Victor Klimov and co-workers at Los Alamos National Laboratory showed that a novel synthesis can produce thin films composed of lead selenide nanocrystals in a titania matrix that exhibit amplified spontaneous emission in the near-IR. Dr. Debbie Jin of JILA/University of Colorado became a 2003 McArthur fellow for her recent work to advance atomic cooling to the study of quantum degeneracy in Bose-Fermi mixtures. Prof. Herschel Rabitz, Princeton University was awarded the Willis E. Lamb Medal for Laser Science and Quantum Optics at the 33rd Winter Colloquium on the Physics of Quantum Electronics for inventing the learning algorithm approach to the coherent control of quantum phenomena. In 2003 four AMOS PIs were named Fellows of the American Physical Society; currently ~70% of the PIs in the program are APS 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. Ultrafast science is now moving into the x-ray regime with enormous potential for following the motion of atoms on the time scale of chemical reactions.

Funding Summary:

Dollars in Thousands

FY 2003	FY 2004	FY 2005 Request
13,379	13,401	13,401

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 49 university grants supporting about 60 students and partially supporting about 59 faculty and senior staff. It also funds 3 programs at national laboratories supporting about 19 senior staff and 5 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 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 and collisions with 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 new accelerator-based sources, 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.

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.