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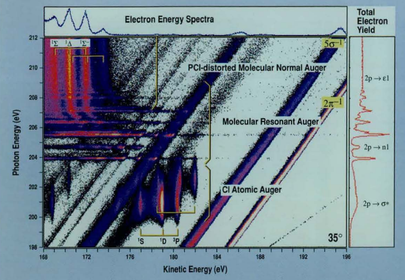
Why Atomic & Molecular Physics?

The scientific motivations for atomic and molecular science fall into two broad categories. *The first is a quest for a deeper understanding of atomic and molecular structures and for new ways of characterizing dynamic many-body interactions.* Many observed phenomena in even relatively simple systems still cannot be successfully treated by sophisticated quantum-mechanical models. The extraordinary characteristics of the ALS coupled with new experimental techniques have created new paradigms for describing many-body interactions in complex systems. For example, experiments using circularly polarized light have shown that particular dynamic electron processes are governed entirely by relativistic interactions. *The second category concerns atomic and molecular phenomena that impinge on other areas of science and technology.* Important questions in sister fields of science often hinge upon a determination of how atoms, molecules, or their ions behave in a specific context or environment. For example, detailed knowledge of the electronic structure of solids or nanostructures must be built upon a thorough understanding of electron-electron interactions in isolated atomic and molecular systems. Since most of our knowledge about the distant universe is carried by photons produced in atomic and molecular processes, the interpretation of astronomical measurements and development of astrophysical models relies heavily upon a quantitative understanding of the electronic structure of atoms, molecules, and their ions, and in particular, of their interactions with photons. The ALS provides powerful means to address atomic and molecular processes in unprecedented detail. There are more examples of the enabling role that atomic and molecular science plays in the development of new technologies (e.g., energy, lasers, biomedical diagnostics, sensors, communications, lighting, and transportation). ■

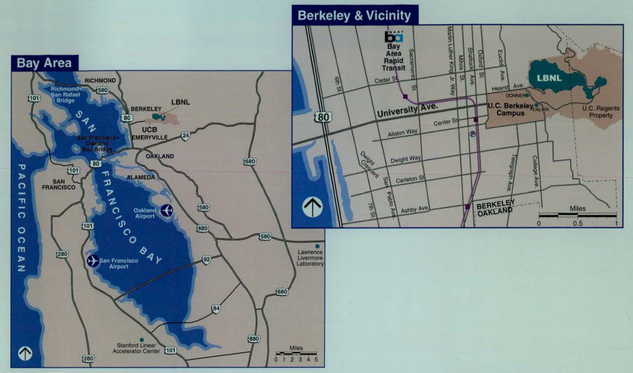


E. Kukk, A. Wills, N. Berrah, B. Langer, J.D. Bozek, O. Nayandin, M. Alshehri, A. Farhat, and D. Cubaynes, *Phys. Rev. A* **57**, R1485 (1998).

COVER IMAGE: Owing to the high brightness of the ALS and to advanced data-acquisition technology, researchers have been able to record two-dimensional electron spectra for the hydrogen chloride (HCl) molecule in the photon-energy range near the threshold for ionization of a tightly bound inner-shell electron associated with the chlorine atom (Cl 2p). With the energy of the photons and the kinetic energy of the ejected electrons as the two axes, the peak positions and their intensities identify several processes, such as the photodissociation giving rise to chlorine atomic Auger, molecular resonant Auger, and normal Auger transitions distorted by post-collision interactions (PCI) labeled in the figure. The diagonal lines labeled $5\sigma^{-1}$ and $2\pi^{-1}$ refer to the absorption of x rays by electrons in outer (valence) molecular orbitals rather than deep inside the chlorine atom, so that these electrons are ejected with high kinetic energy. Following these lines, one can study the interplay between the photoemission and Auger processes.

Getting to the AMF/ALS

The Berkeley Lab is located on a site in the hills directly above the campus of the University of California, Berkeley, and is readily accessible by automobile from anywhere in the San Francisco Bay Area and by limousine or taxi from the San Francisco and Oakland airports. The Bay Area Rapid Transit (BART) system also provides convenient access via its station in downtown Berkeley. Berkeley Lab operates weekday shuttle services: an off-site shuttle between locations around the UC campus and downtown Berkeley to the laboratory and an on-site shuttle.



For More Information

Operating as a user facility, the AMF is open around the year to scientists from academic, industrial, and government laboratories, who may work in collaboration with AMF scientists. Information about the AMF scientific program, Beamline 10.0.1, and the AMF end stations is available by contacting Berrah and Bozek (see below) or visiting the Web at URL: bl10srvr.als.lbl.gov/AMF.htm. For information about how to apply for beam time at the facility through the peer-reviewed Independent Investigator program at the ALS, contact Pepe (see below) or visit URL: www-als.lbl.gov/als/.

AMF Spokesperson	Beamline Contact	Proposal Forms
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ADVANCED LIGHT SOURCE

The ATOMIC and MOLECULAR FACILITY

on BEAMLINE 10.0.1

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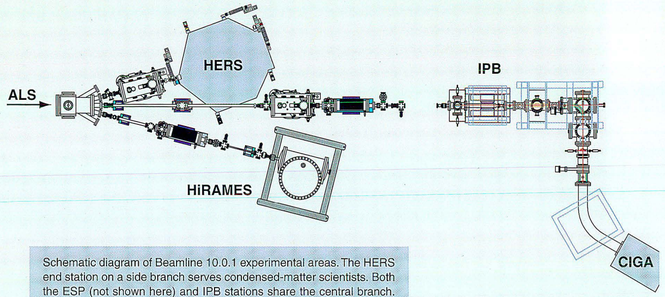
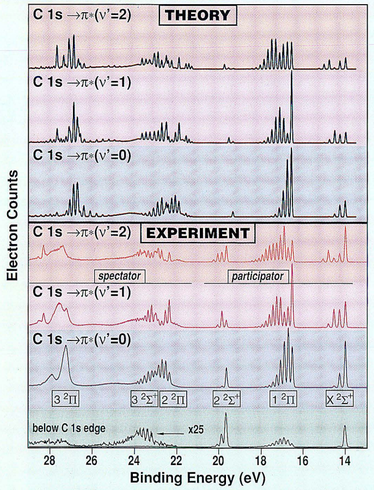
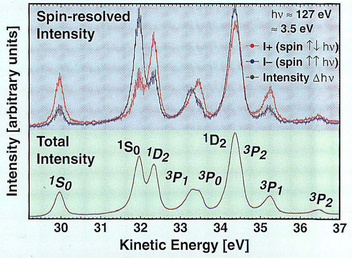


Schematic diagram of Beamline 10.0.1 experimental areas. The HERS end station on a side branch serves condensed-matter scientists. Both the ESP (not shown here) and IPB stations share the central branch. The HiRAMES station occupies the other side branch.



Electron spectra of the C $1s^{-1}$-to-$2\pi^*$ excitation in CO in which the Auger decay to various final ionic states are fully vibrationally resolved. Top three curves are theory, bottom three curves are from HiRAMES. [E. Kukk, J.D. Bozek, W.T. Cheng, R.F. Fink, A.A. Wills, and N. Berrah, *J. Chem. Phys.* **111**, 9642 (1999).]



Xe $N_{4,5}O_{2,3}O_{2,3}$ spin-resolved Auger specta taken with the ESP station at the EPU beamline with circularly polarized light.

The Atomic and Molecular Facility at the Advanced Light Source (AMF/ALS), funded principally by the Office of Basic Energy Sciences of the U.S. Department of Energy, is a "user facility" open to scientists from academic, industrial, and government laboratories. Designed to study highly correlated systems in the gas phase, the AMF combines a new high-resolution undulator beamline (Beamline 10.0.1) with advanced experimental end stations.

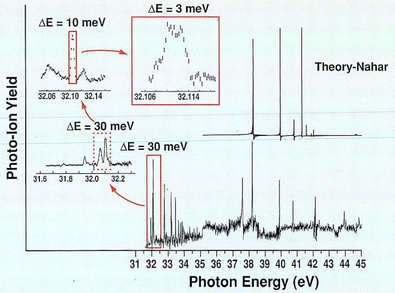
Equipped with a spherical-grating monochromator, Beamline 10.0.1 provides an intense beam of photons at very high spectral resolution over the photon-energy range from 17 eV to 340 eV. The beamline can deliver more than 10^{12} photons per second to the sample at resolving powers (E/ΔE) exceeding 10,000 over most of this photon-energy range. At the expense of resolution, up to 10^{14} photons per second can be obtained over some of this energy range. Alternatively, experimenters can achieve very high resolving power (≈ 64,000) by reducing the monochromator slits and hence the photon flux. The spherical-grating monochromator covers the spectral range with three gratings (380, 935 and 2100 lines/mm). A polarizer (partially funded by the National Science Foundation) comprising four mirrors acting as quarter-wave phase retarders can produce circularly polarized radiation at photon energies from 20 eV to 60 eV. For details of the optical design of the beamline, go to the AMF URL: bl10srvr.als.lbl.gov/AMF.htm.

Downstream from the monochromator exit slits, the beamline has three branches serving experimental end stations. Two of these branches are dedicated to AMF and house three end stations available to AMF users: the High Resolution Atomic and Molecular Electron Spectrometer (HiRAMES) end station, the collinear Ion-Photon Beamline (IPB) end station, and the Electron Spin Polarization (ESP) end station.

Constructed for gas-phase studies of atoms, molecules, and clusters, the High Resolution Atomic and Molecular Electron Spectrometer (HiRAMES) is permanently installed on a side branch of the beamline. The heart of the station is a state-of-the-art Scienta SES-200 electron-energy analyzer capable of 5-meV resolution at 4-eV pass energy. The analyzer is mounted on a chamber that rotates about the photon-beam axis, thereby allowing electron spectra to be obtained at any desired angle relative to the polarization of the photon beam. Gas samples enter a gas cell with differentially pumped openings that allow the photon beam to pass through. An oven is available to heat nonvolatile compounds. The figure showing a high-resolution spectrum of a vibrationally resolved spectrum of the C $1s^{-1}$-to-$2\pi^*$ excitation in CO illustrates the performance achievable with HiRAMES.

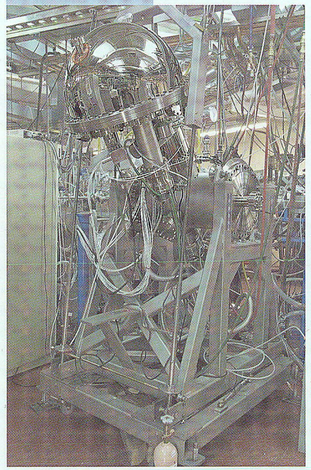
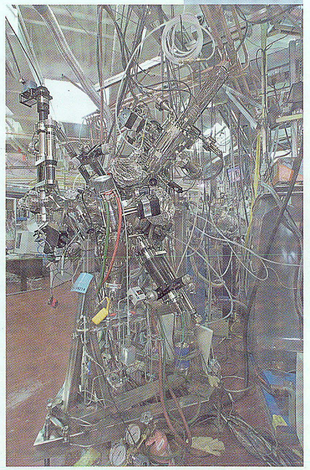
The Electron Spin Polarization (ESP) end station presently allows measurements of the electron spin polarization in free atoms but will be used for the study of molecules and clusters in the future. The ESP end station consists of three electron time-of-flight spectrometers (TOFs) mounted at different angles in a vacuum chamber. Two of the TOFs are equipped with retarding-field Mott-polarimeters, allowing measurements of electron spin polarization components. The third TOF acts as a regular electron spectrometer. Spin-resolved Xe $N_{4,5}O_{2,3}O_{2,3}$ Auger spectra taken at another ALS beamline with circularly polarized light demonstrate the successful commissioning of the ESP station.

The Ion-Photon Beamline (IPB) end station is designed for absolute cross-section measurements and for photo-ion spectroscopy (photoionization and excitation spectra) of singly and multiply charged positive ions, as well as negative ions. A Colutron ion gun apparatus (CIGA) provides an intense source of ions that are photoionized by a collinear beam of VUV or soft x-ray photons. This beamline will also be used to study photoexcitation and photoionization of highly charged ions produced by an electron cyclotron resonance (ECR) source. The high spectral resolution obtained in photoionization measurements of ground-state O^+ confirm the capabilities of the IPB station. ■



Comparison of photoionization measurements at the IPB station and R-matrix theory of S. Nahar [*Phys. Rev. A* **58**, 3766 (1998)] for ground-state O^+. The insets on the left indicate measurements made at increasing photon-energy resolution.

The HiRAMES end station.



The ESP end station.