Investigating Atomic Inner-shell Phenomena with High-energy X Rays

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Background

As pointed out by the FAMOS report to the NRC [1], Atomic Physics is not only a frontier of basic research, but is equally important as an "enabling science" where atomic calculations are used as the basis of other fields. Beyond the hydrogen atom, *all* atomic theory is based on approximation. One of the central themes of modern atomic physics is the interplay between experiment and theory in testing the limits and applicability of those approximations and improving the calculations. In order to best probe the effects of relativity and QED, we need to probe the inner shells of the heaviest atoms and that means high-energy x-ray beams. In this talk, I will present three current examples of such experiments and discuss developments for the future.

Double-K Photoionization in Heavy Atoms

With the advent of modern synchrotron radiation sources providing intense, collimated beams of tunable monochromatic x-rays, there has been increased interest in the investigation of multielectron processes. Beyond the importance of such processes in understanding electron-electron correlations in atoms, they also have significant applications in other fields. For example, they are responsible for the production of satellite structures in extended x-ray absorption fine structure (EXAFS) and x-ray absorption near-edge structure (XANES) studies of materials. The most basic multielectron process is the complete emptying of an atomic K shell in photoabsorption, thus creating a "hollow atom". The APS is unique among U.S. synchrotron light sources for these experiments in that it provides high fluxes of hard x-rays enabling us to reach the double ionization thresholds of all elements.

Following our 1999 observation of the double K-photoionization of molybdenum [2], several groups have exploited modern synchrotron radiation sources to probe the formation and decay of such double K-vacancy states with tunable x rays [3, 4]. Recently, we were able to extend our measurements to the more interesting case of Ag (Z=47). We chose to study silver because of extensive measurements which have been previously carried out using the electron capture (EC) decay of ^{109}Cd in a radioactive source [5] producing hollowed ^{109}Ag. Because one of the electrons is absorbed in the nucleus, there is only a single free electron in the final state, and thus double K-ionization proceeds by a pure shake-off process. Hence, the asymptotic limit is determined independently by the radioactive source measurements. The results are shown in Fig. 1 where in addition to our photoionization data (open circles) we have included the EC data [5] for the asymptotic limit.

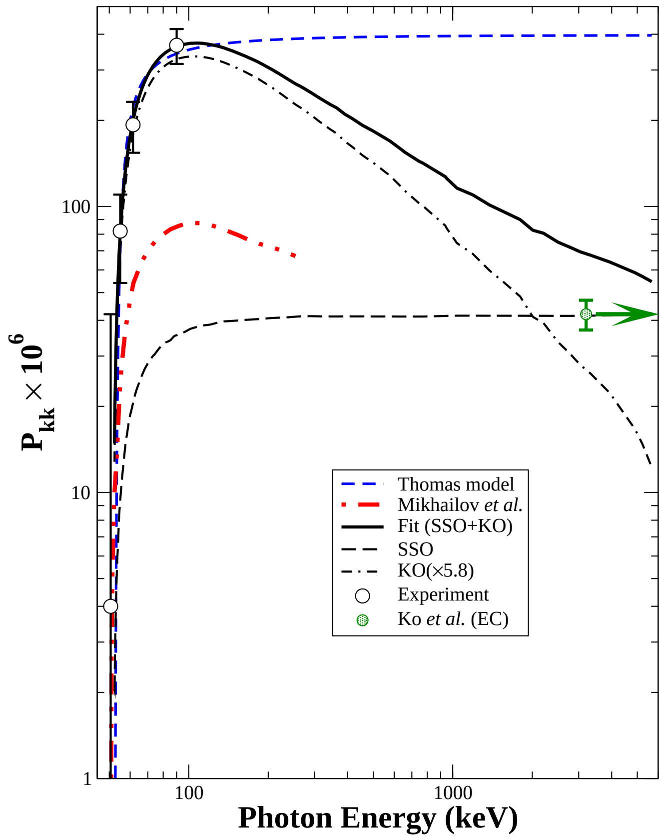

FIG. 1: The ratio of double to single K-ionization of silver as a function of photon energy. The asymptotic limit is indicated by an arrow. The various curves are for different theoretical treatments.

Recently, Rost and his collaborators have suggested a new way to treat this problem [6, 7]. They treat shakeoff (SSO) as the purely quantum mechanical process that it represents – there is no classical analog. The dynamical knockout (KO) is treated quasiclassically and then added *incoherently* to the SSO result. Taking their result and independently scaling their SSO and KO results before

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adding them together, we obtain the solid curve in Fig. 1. These, and other results, have demonstrated that KO may in fact become *more* important with increasing Z than previously believed.

Two-Photon Decays in Au

An inner-shell vacancy in an atom can decay by the simultaneous emission of two photons. Although generally a rare decay mode, 2γ emission is often the dominant mode of decay for dipole-forbidden transitions. Theoretically, it is important because it provides a unique way of testing atomic structure calculations: It is necessary to sum over a complete set of virtual states to desribed this second-order process. Recent interest in theoretical atomic structure is focused on the high-Z region where relativistic and QED effects become important and consequently, high-energy x rays are required for such studies.

Nuclear Excitation by Electron Transition

Nuclear Excitation by Electronic Transition (NEET) is a rare process in which an excited atom relaxes by transferring its excitation energy to the nucleus via a virtual photon. If time is reversed, then it is analagous to internal conversion (where the nucleus de-excites by exciting the atomic configuration) between bound states. Although first postulated in 1973 [8], it was not until quite recently that it was definitively observed at SPring-8 in an experiment on ^{197}Au with 81-keV photons [9]. NEET can only occur when the atomic and nuclear transitions are closely matched in energy and involve the same spin and parity changes. This happens in heavy odd nuclei where the density of low-lying levels ($\lesssim$500 keV) can be high. Consequently, such experiments necessitate high energy x rays to excite the corresponding atomic levels.

Future

An important goal of the double-K photoionization work for the immediate future is to obtain a complete understanding of the cross section from threshold to the asymptotic region. As shown in our work with silver, this means additional measurements in the 200-500 keV region to constrain the theoretical models.

Another related issue is the 2-electron transition in which the double vacancy is filled with the emission of a single photon. Åberg and co-workers obtained a relatively simple expression for the ratio of the intensity of these *correlated hypersatellites* to the more probable satellite transitions [10] which, aside from trivial energy factors, is determined solely by the square of the overlap integral of the K-vacated $2s$ orbital with the relaxed $1s$ orbital. Thus, such a measurement would serve as a particularly simple test of relativistic atomic structure calculations.

Future work at even higher energies will permit study of higher Z atoms where lifetimes are sufficiently prompt to see possible interference with the time-order-reversed decay. Because the 2p level width grows with Z^4 while the satellite-hypersatellite splitting increases slower than Z^2, the level width in uranium is $\sim \frac{1}{5}$ of the hypersatellite splitting. Thus, the hypersatellite and satellite transitions can share energy and one would observe such structure in the region in between. Another interest in high Z atoms is to explore the transition from LS coupling in light atoms to jj coupling at high Z. The hypersatellite ratio $K^h\alpha_1/K^h\alpha_2$ has been demonstrated to be a sesitive probe of the coupling scheme, but measurements in heavy atoms are sorely lacking and it is as yet unknown if this ratio will ever reach the 2/1 value of the diagram line.

The work with two-photon decays also requires higher energies in order to probe the heaviest atoms. For example, no data exist as yet that are sensitive to multipoles beyond $2E1$. Higher multipoles will modify the spectral shape of the continuum spectrum and angular distribution, but such experiments are only feasible in the heaviest atoms. Similarly, one of the frontiers in atomic theory is the investigation of the interplay between relativity and $e-e$ interactions. Measuring the shape of the two-photon continuum as a function of Z can help to test those theoretical treatments.

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