

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Inner-shell photoionization and core-hole decay of Xe and XeF₂¹

STEPHEN SOUTHWORTH, ANTONIO PICÓN, C. STEFAN LEHMANN, Argonne National Laboratory, RALF WEHLITZ, University of Wisconsin, LAN CHENG, JOHN F. STANTON, University of Texas — Molecular effects on inner-shell photoionization and core-hole decay are explored by comparing cross sections and partial ion yields of Xe and XeF₂ from Xe 3d and F 1s subshells in the 660-740 eV range. The Xe 3d-ef continuum shape resonances dominate the total cross sections, but prominent resonances appear in the XeF₂ cross section due to excitation of Xe 3d and F 1s electrons to the lowest unoccupied molecular orbital (LUMO), a delocalized anti-bonding MO. Relativistic coupled-cluster calculations were performed to identify the subshell ionization thresholds, the LUMO resonances and their oscillator strengths. Comparison of the Xe charge state distributions of the atom and molecule show a general shift to lower charge states in XeF₂. The measurements support a model of core-hole decay in which charge is redistributed from Xe to the F ligands and energetic F ions are produced by Coulombic fragmentation.

¹Supported by the Chemical Sciences, Geosciences, and Biosciences Division, Office of Basic Energy Sciences, Office of Science, US Dept of Energy, Contract DE-AC02-06CH11357.

Stephen Southworth
Argonne Natl Lab

Date submitted: 13 Nov 2014

Electronic form version 1.4