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Simulation of Xe_nAr_m Cluster Formation in a Molecular Beam: Comparison with Photoelectron Spectroscopy FRANCOIS G. AMAR, THOMAS J. PRESTON, Department of Chemistry, University of Maine, Orono, ME 04469-5706 — We perform direct MD simulations of the formation of mixed Xe_nAr_m clusters (500<n+m<3000) in a supersonic beam as a function of initial beam conditions. We then model the $4d_{5/2}$ (Xe) and $2p_{3/2}$ (Ar) core hole photoelectron spectra of these clusters and compare them to the experimental spectra of Tchaplyguine *et al*[1]. The predicted spectra are calculated as the sum of final state energy shifts of the ionized atoms (within the cluster) relative to the isolated gas phase ion using a self-consistent polarization formalism. We use the results of our earlier calculations on pure argon and xenon clusters [2] to determine the appropriate inelastic mean free path value for the signal electrons leaving the mixed clusters. These results allow us to gain a refined understanding of the size, stoichiometry, and core/shell structure of these mixed clusters. [1] M. Tchaplyguine, *et al*, Phys. Rev A **69**, 031201 (2004); [2] F. Amar, *et al*, JCP **122**, 244717 (2005).

Jacques Amar
Dept of Physics, University of Toledo

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