DYNAMICS OF THE "EXCESS" ELECTRON IN SMALL WATER CLUSTER ANIONS

JOHN M. HERBERT and MARTIN HEAD-GORDON, *Department of Chemistry, University of California, Berkeley, CA 94720*.

Dynamics subsequent to electron attachment in small $(H_2O)_n$ clusters ($n \leq 6$) are simulated by *ab initio* molecular dynamics. Unlike previous pseudopotential-based simulations of water cluster anions, the use of electronic structure potentials in the present work allows for quantitative prediction of photoelectron spectra, while dynamical simulation of the molecular orbitals allows us to distinguish between surface-bound states and internalized states of the unpaired electron, which can interconvert as the cluster geometry changes. We attempt to assign and interpret the observed photoelectron spectra for $(H_2O)_4^-$, $(H_2O)_5^-$, and $(H_2O)_6^-$ in terms of stable isomers versus available autodetachment channels.