FIRST-PRINCIPLES QUANTUM-CHEMICAL SIMULATIONS OF THE HYDRATED ELECTRON

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I will discuss our group's ongoing efforts to elucidate the structure and dynamics of hydrated-electron clusters, $(H_2O)_n^-$, using *ab initio* quantum chemistry. Theoretical techniques include first-principles molecular dynamics and Monte Carlo simulations, as well as detailed analysis of the wave function associated with the "excess" electron. We apply these methods to predict and interpret both vibrational and photoelectron spectra of $(H_2O)_n^-$.