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Theoretical Studies of Negatively Charged Water Clusters: The Role of Polarization and Dispersion for Electron Binding[1]

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A quantum Drude oscillator model is used to characterize negatively charged water clusters as large as $(H_2O)_{24}^-$. The Drude model allows for inclusion of electron correlation effects between the excess electron and the electrons of the water molecules, at a fraction of the computational cost of all-electron *ab initio* methods. Application of the Drude model to $(H_2O)_6^-$ demonstrates that there are many isomers with small electron binding energies that are more stable than the species with double acceptor water monomers that dominate under experimental conditions and that have electron binding energies near 0.45 eV. The talk will also explore the connection between the Drude model and more traditional polarization models used in describing the interaction of excess electrons with water. We show that a series of "polarization" models can be derived from the Drude model, by carrying out an adiabatic separation between the excess electron and the Drude degrees of freedom. It is found that the polarization and Drude models give similar electron binding energies for species in which the excess electron experiences large electrostatic attraction, but that the polarization models significantly overbind the excess electron in cases where the electrostatics play only a small role.

[1]In collaboration with Albert DeFusco, University of Pittsburgh and Thomas Sommerfeld, Southeastern Louisiana University.