Molecular Simulation of Water and Aqueous Solutions

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In this talk, we describe our efforts to develop intermolecular potentials for water and aqueous solutions. We have had as our goal the development of a polarizable model for water whose bare dipole moment matches that of the isolated water molecule (1.85D), that accurately predicts the structure of water at ambient and supercritical conditions, and that reproduces thermodynamic and dielectric behavior, including the phase envelope. We will describe the evolution of our model to the latest version, the Gaussian charge polarizable model (GCPM), which achieves many of the goals we set for our model. We will also outline our recent efforts to extend this model to solutions of ionic and hydrophobic solutes.