

Abstract Submitted
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A self-consistent polarizable electron water potential: applications to clusters and bulk LEIF JACOBSON, the Ohio State University — We have recently re-parameterized the electron–water potential due to Turi and Borgis [J. Chem. Phys.**117**, 6186 (2002)] to be used with the polarizable water potential AMOEBA for use in hydrated electron simulations. In our model the single electronic wave function polarizes the water molecules and vice versa in a fully self-consistent manner. Comparison to binding energies and relative energetics of $(\text{H}_2\text{O})_n^-$ isomers (with $n < 33$) to *ab initio* results show a significant increase in accuracy over the previous parameterization which used a fixed charge water model. The relative importance of polarization in various binding motifs as well as cluster and bulk molecular dynamics simulations will be presented. The simulated optical absorption spectra will also be discussed.

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