RE–OPTIMIZATION OF AN ELECTRON–WATER PSEUDOPOTENTIAL

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In order to assess the role of self-consistent polarization in simulated properties of electron–water clusters and the experimental extrapolation of VEBE (Vertical Electron Binding Energies) to their bulk counterparts we have previously parameterized an electron–water pseudopotential similar to that most commonly used. This potential was shown to perform very well in reproducing VEBE's of a large database of clusters as well as reproducing relative isomer energies of small clusters as compared to MP2 predictions. However, when applied to study the dynamics of large systems (greater than 20 water molecules) this potential yielded a diffusely bound, interpenetrating, unstructured picture of the hydrated electron, inconsistent with chemical intuition and experimental results predicting a well defined solvation cavity. We re–evaluate assumptions that went into our previous parameterization, in particular the repulsive potential that arises when casting the true many–electron problem into an effective one–electron problem. Cluster and bulk binding energies as well as electronic absorption spectra will be investigated.