DESCRIBING THE HYDRATED ELECTRON WITH A POLARIZABLE ELECTRON-WATER PSEUDOPOTENTIAL

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We have constructed a one-electron pseudopotential that treats the mutual polarization of an excess electron with a water bath in a self-consistent fashion. This potential is able to reproduce MP2-quality vertical binding energies of anionic water clusters with an average error of less than 0.1 eV. We are also able to reproduce the bulk optical absorption spectrum of the aqueous electron where we find that the many-electron response of the water bath is important in describing the lineshape of this spectrum. The binding energy and absorption spectrum maximum have been important experimental observables in studies of anionic water clusters and so our potential is well suited to address the structural complexity of these systems. We reconstruct a diagram of vertical binding energy versus inverse cluster size in order to investigate the extent to which our model is able to reproduce photoelectron experimental data for anionic water clusters for n=20-200, as well as provide insight into the binding motifs of these clusters.