IMPORTANCE OF SELF-CONSISTEN POLARIZATION IN ELECTRON WATER PSEUDO-POTENTIAL

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The hydrated electron has been a species of interest in chemical physics for many decades and single electron pseudo-potentials have allowed calculation of large system properties of this species. Due to stabilization of unfavorable neutral water geometries on the anion potential energy surface polarization is known to play an important role in determining the energetics of such systems. Pseudo-potentials applied to large systems have largely ignored this fact. We construct a new electron-water pseudo-potential which treats polarization in a self-consistent manner. Using a grid based representation of the electron and classical nuclei we investigate the effect of the inclusion of self consistent polarization on structural and energetic distributions.