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Beyond a single solvated electron: Hybrid quantum Monte Carlo and molecular mechanics approach DMITRY ZUBAREV, UC Berkeley, Department of Chemistry, GARY CLARK, TERESA HEAD-GORDON, UC Berkeley, Department of Bioengineering, WILLIAM LESTER, UC Berkeley, Department of Chemistry — A hybrid computational approach combining quantum Monte Carlo and molecular mechanics (QMC/MM) has been recently developed for an accurate treatment of electron correlation in systems that require a large number of explicit solvent molecules. Here, QMC/MM is utilized to address the issue of binding of two excess electrons to water clusters of medium-to-large size. Such systems are relevant to the studies of interaction of excess electrons with solvent molecules during electron-energy transfer in medium. A modeling strategy is proposed that combines polarizable force field simulations and density functional theoretical calculations for geometries and binding energies of dianionic clusters, and QMC/MM calculations for refined binding energies. The possibility of stable doubly charged anionic water clusters is demonstrated. The study explores binding properties of various structural motifs and how stability towards spontaneous electron detachment depends on cluster size. Applicability of QMC/MM to the studies of metastable systems is discussed.

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