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Distinguishing cavity and non-cavity solvation structures of the hydrated electron

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Solvated electrons in aqueous solution are a prototypical low dimensional quantum system in interaction with a fluctuating many-body environment. Despite substantial theoretical and experimental effort, conflicting views prevail regarding the hydration structure of electrons in water, where cavity and non-cavity solvation structures have been suggested. We present first principles molecular dynamics simulations of the electron localization dynamics in liquid water, employing hybrid-meta-GGA and hybrid-GGA density functionals that both provide an excellent description of the liquid water structure. Nevertheless, characteristic differences occur regarding the localization dynamics and solvation structure of excess electrons. We identify perturbations of the local hydrogen bond structure of water due to the interaction with the excess charge that give rise to specific signatures in transient radial distribution functions. Respective signatures in simulated scattering patterns are compared to preliminary data obtained in a liquid phase UED early science campaign at SLAC. The results shine light on the coupling mechanism of the aqueous electron with its environment and provide microscopic insight into the dynamics of polaron formation in disordered condensed matter systems.

Keywords

Hydrogen bonds, ab-initio molecular dynamics simulations, solvated electron, liquid phase ultrafast electron diffraction

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