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Optical Spectrum of the Hydrated Electron in Supercooled and Supercritical Water and Ice DAVID BARTELS, ERICA PRICE, YIQUI DU, Notre Dame Radiation Laboratory — Simulation of the hydrated electron optical spectrum has been the goal of a generation of researchers, and was apparently achieved within the last decade using a one-quantum-electron/pseudopotential/classical water MD modeling strategy. The temperature dependence of the spectrum (red shift at elevated temperature) was reported to be actually the effect of water bulk density. The red shift in simulation was linear in the inverse density. Spectra of the hydrated electron recorded in our laboratory in supercritical water strongly disagree with the simulation result, in that there is very little spectral change for a factor of six change in water density, from 0.1 to 0.6 g/cc at 375°C. A new result presented here concerns the spectra in supercooled water, which can be compared with spectra in water at higher temperature at the same bulk density. In this comparison, density of the water very clearly does not determine the position of the absorption maximum—the temperature does. The one-quantum-electron/pseudopotential/classical water MD methodology clearly lacks some critical aspects of the real water-electron interaction. A comparison of the electron solvated in supercooled water or in ice at the same temperature shows virtually the same shape on the blue side, but a much narrower bandwidth on the red side in ice relative to water.

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