Hydrogen bond dynamics in liquid water from quantum molecular dynamics

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An *ab initio*-based, polarizable water force field is employed in combination with the centroid molecular dynamics method to investigate the ultrafast rearrangement of the hydrogen-bond network at a quantum-mechanical level. In particular, the orientational dynamics of dilute HOD molecules in H_2O and D_2O is analyzed as a function of the temperature, and the results are discussed in connection to the experimental linear and two-dimensional infrared spectra. The importance of nuclear quantum effects is quantitatively assessed, and a comparison with the results obtained from classical simulations with point charge, empirical force fields is presented.