A Reactive Force Field Molecular Dynamics Simulation for the Lifetime of Hydrogen Bonds in Supercritical Water

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Supercritical water is receiving considerable attention in various applications, including the extraction of bioactive compounds in green plants, the oxidation of organic pollutants, and the gasification of low-rank coal. It is well known that hydrogen bond plays an important role in the physical and chemical properties of supercritical water. In the present work, reactive force field molecular dynamics simulations are performed to investigate the lifetime of hydrogen bonds in supercritical water. 1000 water molecules are simulated under NPT ensembles for 0.25 ns. The temperature ranges from 700 K to 1000 K and the pressure ranges from 25 MPa to 50 MPa. The hydrogen bond is determined by a geometric criterion and the lifetime is calculated with a tracking method. It is shown from the simulation results that the hydrogen bond in supercritical water experiences the dynamic process of forming, cracking, re-bonding, and exchanging within the time span of femtosecond. The calculated average lifetime of hydrogen bonds ranges from 17.5 to 24.1 fs. The lifetime decrease with the increase of temperature as well as the increase of pressure and is primarily temperature dependent. Charge analysis reveals that with an increase of temperature, the amount of charge of the donor hydrogen atom and the receptor oxygen atom decreases, which results in a weaker electrostatic interaction within a hydrogen bond.