Molecular Dynamics Simulation on the Dynamical Behavior of the Water Monomer inside a Single-Walled Carbon Nanotube

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The dynamical behavior of the water monomer inside a single-walled carbon nanotube (SWNT) is investigated by the molecular dynamics simulation method. The water monomer put initially at random into a SWNT is perturbed by the breathing, lengthening, and shortening modes of a SWNT and moves along the z-axial direction. While achieving the steady state, the water monomer remains the optimal geometrical distance, which is the mean value, and stays closer to the wall of a SWNT instead of to keep nearly the z-axial center of a SWNT. For a (5,5) SWNT with 6.8 Å in diameter, the optimal geometrical distance is 2.56 Å; however, for a (10,10) SWNT with 13.57 Å, it is 3.69 Å. In the present study, the dynamical behavior and motion mechanism of the water monomer, which is inside a SWNT, stirred by the thermal noise of a SWNT are studied. Moreover, the scale, chiral, and temperature effects of a SWNT containing the water monomer are also evaluated.