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**Low dimensional molecular dynamics of water inside a carbon nanotube** JUNICHIRO SHIOMI, The University of Tokyo, YUAN LIN, GUSTAV AMBERG, Royal Institute of Technology (KTH), SHIGEO MARUYAMA, The University of Tokyo — While carbon nanotubes (CNTs) have attracted a number of researches as the key building blocks for nanotechnology, they have also caught attentions as ideal materials that realize quasi-one-dimensional channel environment, a key system in bioscience. Such materials stimulate studies in fluid dynamics under low dimensional confinement, which is restricted and departs significantly from that in three-dimension. The current study serves to explore such atomic scale dynamics by performing a series of molecular dynamics (MD) simulations on water confined in a CNT with a diameter of the order of 1 nm. The MD simulations have successfully probed the phase transition of a water cluster confined in a CNT to an ice-nanotube with anomalous diameter dependence. It has also been applied to investigate the possibility of transporting water through a CNT by a temperature gradient. In this study, we particularly highlight the dielectric properties of water confined inside a CNT. The confinement gives rise to strongly anisotropic dielectric relaxation, where the relaxation becomes faster and slower in the cross sectional and axial directions, respectively. The diameter dependences of the dielectric properties are discussed in connection with water dynamics and structures in quasi-one-dimension.

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