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Molecular dynamics simulation of water inside and outside carbon nanotubes JOHN THOMAS, ALAN MCGAUGHEY, Carnegie Mellon University — The behavior of liquid water inside and outside 1.1 nm, 2.8 nm, 6.9 nm, and 10 nm diameter armchair carbon nanotubes (CNT) is predicted using molecular dynamics simulation. The effect of CNT diameter on mass density and distribution, molecular orientation, and the self-diffusion coefficient tensor are identified for both the confined and unconfined fluids. Within 1 nm of the CNT surface, unconfined water molecules assume a spatially varying density profile. The molecules distribute non-uniformly around the carbon surface and align parallel to the CNT centerline. This results in a non-uniform self-diffusion coefficient tensor near the solid. The behavior of the unconfined water molecules is invariant with CNT diameter. The behavior of the confined water is correlated to CNT diameter. Inside the 10 nm tube, the molecular behavior is indistinguishable from that of the unconfined fluid. Within the smaller tubes, surface curvature effects force water molecules away from the surface and extend the influence of the solid. These spatially varying static properties influence the self-diffusion tensor within the tube.

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