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Subcontinuum water transport through carbon nanotubes JOHN THOMAS, ALAN MCGAUGHEY, OTTOLEO KUTER-ARNEBECK, Carnegie Mellon University — The structure and flow of water inside carbon nanotubes (CNTs) with diameters ranging from 0.86 nm to 1.66 nm are examined using molecular dynamics simulations. A sample of each CNT is placed between two water reservoirs, and a pressure difference is established between the reservoirs to induce flow through the CNTs. In CNTs with diameters greater than 1.4 nm, the axial distribution of water molecules is uniform and the molecules at the center of the CNT display hydrogen bonding characteristics similar to those found in bulk water. In CNTs with diameters less than 1.4 nm, both the axial distribution of water molecules and the hydrogen bonding characteristics at the center of the CNT vary with tube diameter. The diameter-dependent behavior leads to mass transport phenomena that cannot be explained using continuum fluid mechanics. For example, under the same pressure gradient, flow velocity is found to increase with decreasing CNT diameter. The effect of water entering and exiting the CNT from the reservoir is also examined.

John Thomas
Carnegie Mellon University

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