Enhancement Flow in Nanoconfined Water

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We investigate through non-equilibrium molecular dynamic simulations the flow of core-softened fluids inside nanotubes. Our results reveal a anomalous increase of the overall mass flux for nanotubes with sufficiently smaller radii. This is explained in terms of a transition from a single-file type of flow to the movement of an ordered-like fluid as the nanotube radius increases. The occurrence of a global minimum in the mass flux at this transition reflects the competition between the two characteristics length scales of the core-softened potential. Moreover, by increasing further the radius, another substantial change in the flow behavior, which becomes more evident at low temperatures, leads to a local minimum in the overall mass flux. Microscopically, this second transition results from the formation of a double-layer of flowing particles in the confined nanotube space. These special nano-fluidic features of core-softened particles closely resemble the enhanced flow behavior observed for liquid water inside carbon nanotubes.

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