Thermal Transport of Confined Water in Nanotubes using Molecular Dynamics Simulations

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Nanoscale confinement can qualitatively alter liquid structure and transport, as the surface-to-volume ratio is high and solid-liquid interfacial effects become dominant. In carbon nanotubes, water can adopt distinct molecular organizations such as single-file and layered states, which strongly influence axial thermal transport. While confinement geometry has been recognized as a key control parameter [1], the role of nanotube surface wettability in thermal transport remains less established, despite its direct impact on interfacial interactions and molecular structuring [2].
To study these wall-induced effects on liquid structure and thermal conductivity, we performed non-equilibrium molecular dynamics simulations of water confined in nanotubes with different surface wettabilities. We find that more hydrophilic nanotubes lead to higher thermal conductivity. Under hydrophilic conditions, molecular diffusion is suppressed and the local density increases, indicating a more solid-like character that facilitates axial heat transport.

Keywords:
Nanoconfinement: Wettability: Molecular dynamics

References:

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