Barriers to Superfast Water Transport in Carbon Nanotube Membranes

Carbon nanotube (CNT) membranes hold the promise of extraordinary fast water transport for applications such as energy efficient filtration and molecular level drug delivery. However, experiments and computations have reported flow rate enhancements over continuum hydrodynamics that contradict each other by orders of magnitude. We perform large scale molecular dynamics simulations emulating for the first time the micrometer thick CNTs membranes used in experiments. We find transport enhancement rates that are length dependent due to entrance and exit losses but asymptote to 2 orders of magnitude over the continuum predictions. These rates are far below those reported experimentally. The results suggest that the reported superfast water transport rates cannot be attributed to interactions of water with pristine CNTs alone.

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