Computational design of single- and multi-layer Transverse Flow Carbon Nanotube membrane using empirical molecular dynamics

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Abstract

Using molecular dynamics (MD), we computationally designed the Transverse Flow Carbon Nanotube (CNT) Membrane (TFCM) and show that this simple membrane design is highly efficient. In terms of desalination performance, the resulting TFCM membrane offers permeability a few orders of magnitude larger than conventional polymeric reverse osmosis membrane, and more than two times that of two-dimensional graphene. In this presentation, we introduce the TFCM. TFCM is made by stacking CNTs horizontally one on top of another, forming hourglass slits that allow fast water passage while blocking salt ions. The single layer TFCM is formed by only one layer of stacked CNTs, and the critical slit size that separates neighbouring CNTs have to be kept at 0.33nm to effectively reject salt. By multilayering, the slit size between neighbouring CNTs can increase to beyond 1nm while still effectively rejecting salt. This increase in slit size compensates the permeability reduction due to multilayering, allowing multilayer TFCM to permeate water as fast as single layer TFCM. Our MD work provides computational evidence that such outer-flow CNT membrane can be a simple and effective design for future low dimensional materials membrane.

Keywords: Molecular dynamics, low dimensional materials, membrane, desalination, carbon nanotubes, computational design