Atomistic Simulation of Desalination

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In this research, we investigate the desalination capacity of three-dimensional (3D) carbon nanostructures using molecular dynamics simulations. 3D carbon nanostructures proposed here will filter seawater efficiently because of their multiple layers with holes of tunable sizes. The structure is designed to be flexible, allowing mechanical deformation during daily use. The 3D carbon nanostructure will still possess high thermal conductivity, enabling easy recycle through a simple heating process. Here, we employ LAMMPS, Large-scale Atomic/Molecular Massively Parallel Simulator distributed by Sandia National Laboratories to measure salt ion flux through 3D carbon nanostructure membrane. Pillared graphene structures (which is consisted of graphene floors and carbon nanotube (CNT) pillars) are selected as the representative 3D carbon nanostructure. An initial 3D carbon nanostructure was constructed using custom MATLAB program. The solvation and ionization of a 3D carbon nanostructure were accomplished by using Visual Molecular Dynamics (VMD); ions of sodium (Na^+) and ions of choline (Cl^-) were placed into solution to simulate saltwater. Combined Airebo and TIP4P force field was used to define interatomic potential between atoms. During the simulation, it was observed that water molecules passed through CNT pillars that connect graphene floors efficiently while salt ions were blocked because of the limited diameter of CNT pillars. The results obtained in the present research will accelerate the development of more efficient and environmental friendly solution for the desalination of seawater.

Keywords: Molecular dynamics, seawater filter, carbon nanostructure