Molecular Dynamics Simulation and Experimental Fabrication of Nanoporous Graphene Membranes for Optimal Water Permeability in Reverse Osmosis Desalination

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Nanoporous graphene membranes have the potential to solve the problem of a dwindling supply of fresh water that affects nearly half the world's population by enabling low cost, efficient desalination of seawater. Modern reverse osmosis desalination plants are expensive, environmentally disruptive and consume large amounts of energy. Due to their single-atom-thickness, these membranes have demonstrated to be highly permeable. LAMMPS molecular dynamics simulation software was utilized on a 100,000 core-hour supercomputer allocation to model nanoscale water filtration across nanoporous graphene for thirty 10 nanosecond trials. Optimal water permeability of these membranes was determined to be 125 L cm^-2 d^-1 MPa^-1 at a 6.2% porosity for adequate mechanical stability in reverse osmosis by variation of five porosities and hydrogen or hydroxyl functional pore linings. This permeability is 5,180 times greater than common thin-film and 20 times greater than ultrafiltration membranes. Nanopores were experimentally fabricated in 45 samples of mono- and bilayer graphene sheets, after preparation of membranes by graphene transfer onto three substrates and defect-sealing via atomic layer deposition and interfacial polymerization. Gallium ion bombardment with oxidative etching and oxygen plasma etching were respectively used to create 0.4 nm and 1 nm pores at densities between 10^12 and 10^13 pores per square centimeter. Samples were produced at up to 20 square centimeters in area and were characterized by transmission and scanning electron microscopy, as well as Raman and x-ray photoelectron spectroscopy. Three water transport measurements were conducted per sample and demonstrated membrane permeability of up to 50 L cm^-2 d^-1 MPa^-1, corroborating theory at that density by 92%.

Awards Won:

First Award of $5,000

NASA: Second Award of $750