NANYANG TECHNOLOGICAL UNIVERSITY SINGAPORE
Environmental Process Modelling Centre
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Design & Development of 2D Nanomaterial-Based Membranes for Water Desalination: Molecular Dynamics (MD) Simulation

Why MD simulation?

Owing to the structure being one atom-thick, 2D nanomaterials have exhibited huge potential in membrane desalination technologies. MD simulation enables the possibility to construct and examine such nanostructured membranes by revealing the atomistic behavior of water inside the nanostructure.

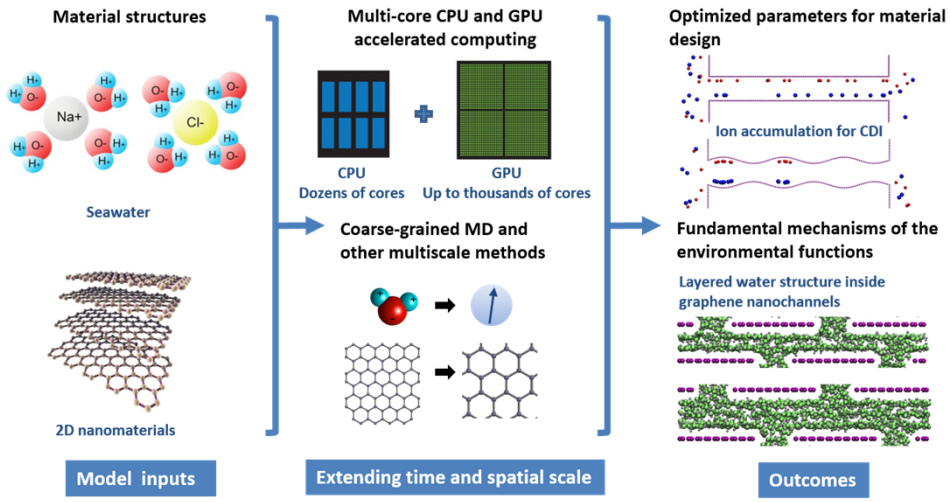

Fig. 1. Schematic of MD simulation processes.

2D nanostructured membranes for desalination

Reverse osmosis (RO)

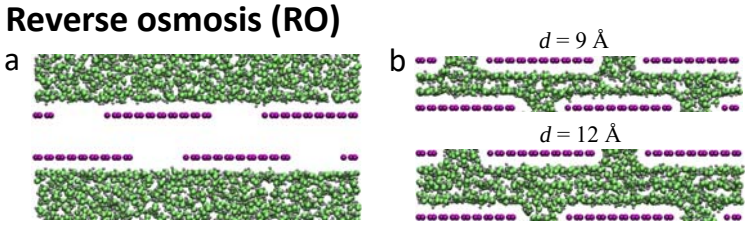

Fig. 2. (a) Schematic of RO desalination using a bilayer graphene membrane and (b) the layered structure of H_2O molecules inside the membrane.

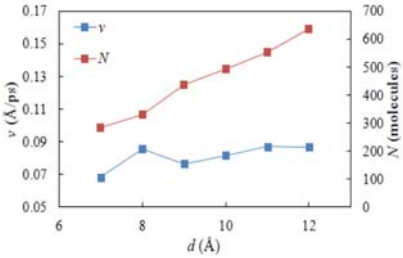

Fig. 3. Dependence of the number and velocity of H_2O molecules on the interlayer distance.

- Permeation flux of water inside bilayer graphene (GE) is close to that of monolayer porous GE, while achieving higher salt rejection.
- Increasing the pore density of bilayer GE can significantly improve the water flux without sacrificing the salt rejection.
- The interlayer distance affects the permeation flux of bilayer GE in a nonmonotonic manner, determined by the evolution of the layered structure of water molecules.

Forward osmosis (FO)

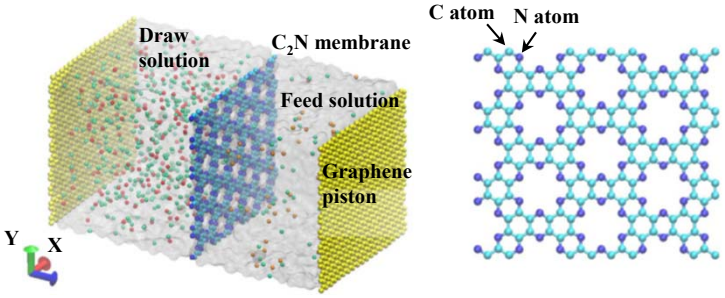

Fig. 4. Schematic of FO desalination (left) using a strained single-layer C_2N membrane (right).

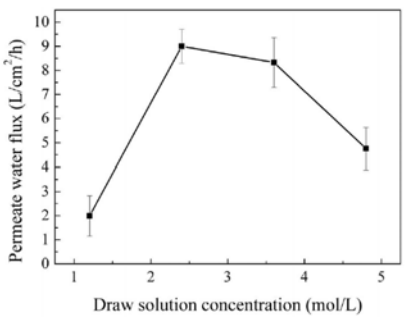

Fig. 5. Effect of osmotic pressure difference on the permeation flux.

- At 4% strain, the membrane becomes permeable only to water molecules.
- At 12% strain and 338 K, high flux of 14.36 $Lcm^{-2}h^{-1}$ is obtained.
- The permeation water flux shows a nonmonotonic dependence on the osmotic pressure difference.