

MOF-Based Nanoporous Membranes for Seawater Desalination

BCKGROUND

What is MOF?

Metal-organic frameworks (MOFs) are a new class of porous solid materials, which are constructed by metal ions/clusters and organic linkers (Fig. 1). The pore size of MOFs can be rationally adjusted from several angstrom (Å) to several nanometer (nm). Therefore, MOFs can be designed and prepared as nanoporous membranes to allow the permeation of water molecules while rejecting larger hydrated salt ions (Fig. 2).

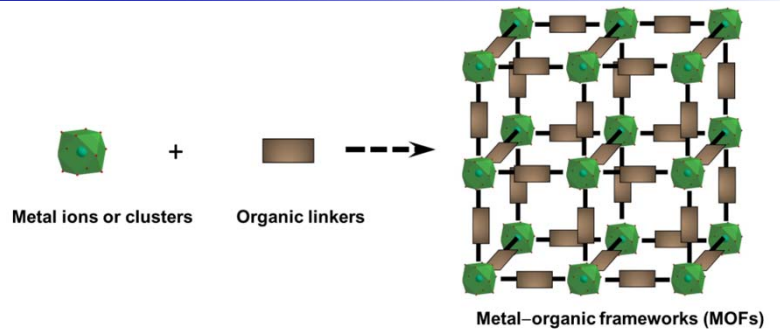


Fig. 1. Schematic illustration of the structure and component of MOFs.

MOLECULAR DYNAMICS (MD) SIMULATION

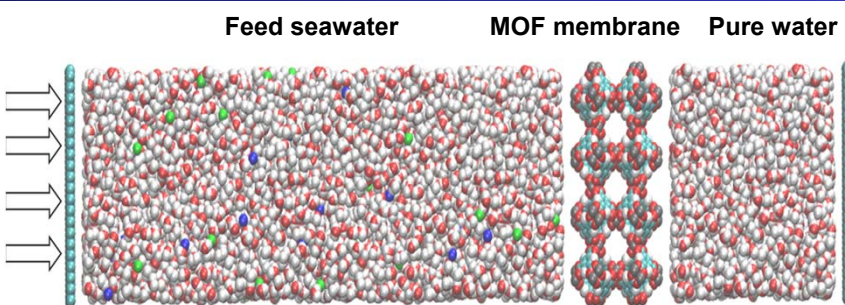


Fig. 2. MD simulation system for reverse osmosis through a MOF membrane. Cyan, red, white, grey, green and blue represent C, O, H, Cu, Na⁺ and Cl⁻, respectively.

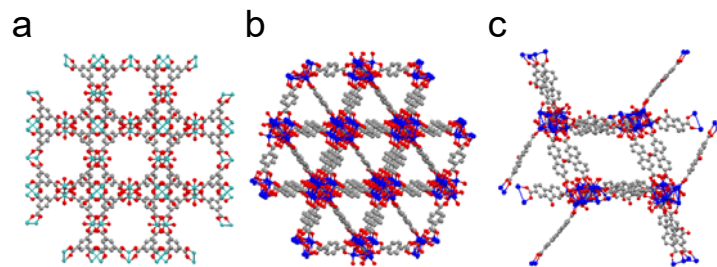


Fig. 3. Three types of MOF structures with different pore sizes: (a) HKUST-1, (b) UIO-66 and (c) UIO-67. Green, blue, red, and grey represent Cu, Zr, O and C, respectively.

MATERIALS FABRICATION AND CHARACTERIZATION

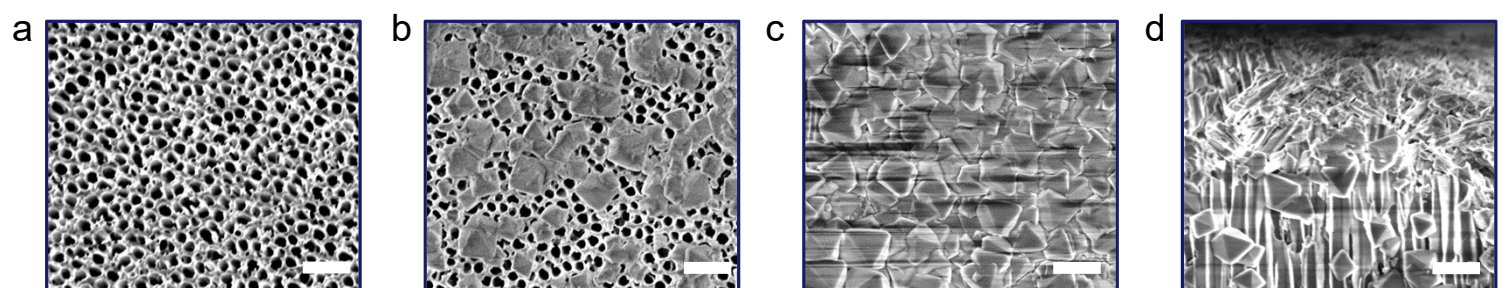
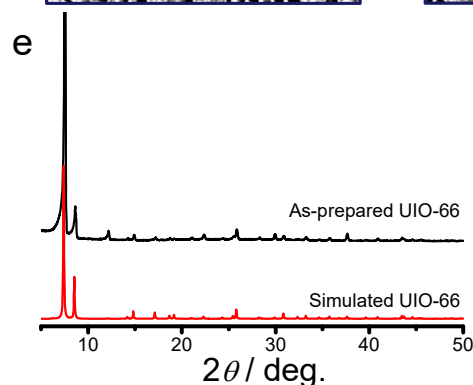


Fig. 4. SEM images of UIO-66 membranes on the Al₂O₃ substrate: (a) porous substrate; (b) discontinuous UIO-66; (c)-(d) continuous UIO-66 in the top and cross-sectional views, respectively (scale bar: 1 μm). (e) XRD patterns of UIO-66.



SUMMARY

- MD simulation was used to investigate nanoporous MOF materials (HKUST-1, UIO-66 and UIO-67) as desalination membranes.
- MOF-based membranes were fabricated to investigate the desalination performance and verify the simulation results.