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Synergistic effects of crystal structure and surface chemistry of stacked graphene-oxide membranes on the water-permeation mechanism

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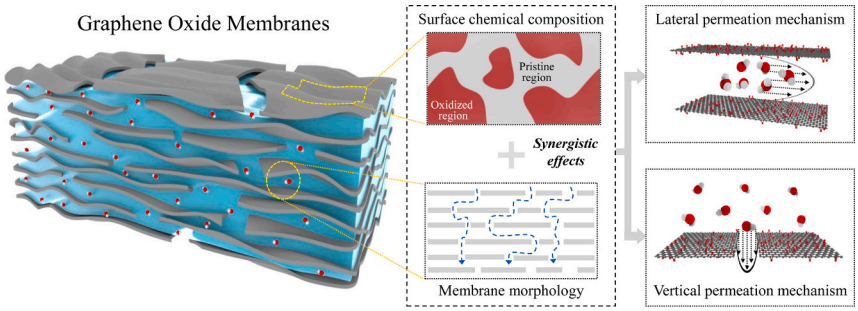
GRAPHICAL ABSTRACT



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ABSTRACT

Stacked graphene-oxide (GO) membranes have been reported to have promising potential for desalination. One key issue in the development of such membranes is understanding the atomistic water-permeation mechanism determined by the highly variable nature of GO (including membrane morphology, surface chemistry, osmotic pressure, and surface area). To clearly understand this variability, not only individual but also synergistic effects, i.e., the nonlinear cumulative effects of membrane properties, should be investigated. Hence, this paper explores how lateral and vertical permeation mechanisms differ with changes in the morphology and surface chemistry, either discretely or simultaneously, using both experiments and simulations. Experiments reveal that the GO water-permeation performance is dominated by the heterogeneous structural and chemical nature of GO. To investigate individual and synergistic effects on water dynamics, we performed molecular-dynamics simulations. The synergistic effects were more marked on the lateral permeation mechanisms than on the vertical mechanism in GO membranes. When the membrane nanochannels had a narrow intersheet distance or no gap overlap, the lateral permeation mechanism was found to be completely different owing to the interplay between these properties.

Abbreviations: ABF, Adaptive-biasing-forcing; CCD, Charge-coupled device; GK, Green-Kubo; GO, Graphene-oxide; LAMMPS, Large-scale Atomic/Molecular Massively Parallel Simulator; MD, Molecular-dynamics; MSIP, Ministry of Science, ICT, and Future Planning; NVT, Number of particles, volume, and temperature; OPLS, Optimized potential for liquid simulations; OVaaT, One-variable-at-a-time; OVITO, Open Visualization Tool; PMF, Potential mean force; RO, Reverse osmosis; XPS, X-ray photoelectron spectroscopy

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