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Gas permeation through double-layer graphene oxide membranes: the role of interlayer distance and pore offset

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Abstract

Hierarchically stacked graphene oxide (GO) membranes have sparked considerable interest due to their prominent separation performance; however, the underlying separation mechanisms remain elusive. In this study, we conducted molecular dynamics (MD) simulations to explore the role of interlayer distance and pore offset in gas (H₂, CH₄, N₂ and CO₂) permeation through double-layer GO membranes. Gas permeance is found to increase with the interlayer distance and pore offset until the interlayer distance exceeds a critical value. With elongating the interlayer distance and pore offset, a sieving effect occurs to overcome preferential adsorption and dominates the transport in mixed H₂/CO₂, resulting in selective permeation shifting from CO₂ to H₂. This simulation study provides mechanistic insight into gas permeation through layered GO membranes, and would facilitate the design of new GO membranes for high-performance gas separation.

Keywords: graphene oxide membrane; molecular simulation; gas separation

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