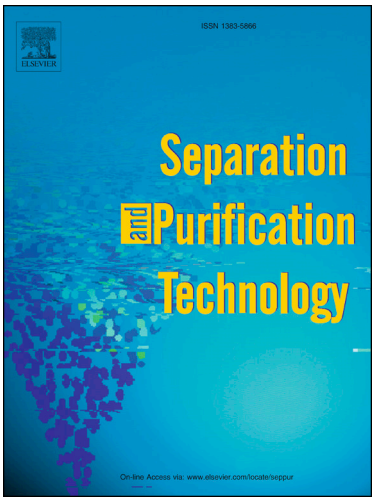

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Quan Liu, Krishna M. Gupta, Qisong Xu, Gongping Liu, Wanqin Jin

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

Quan Liu[a], Krishna M. Gupta[b], Qisong Xu[b], Gongping Liu[a,*], Wanqin Jin[a,*]

[a]State Key Laboratory of Materials-Oriented Chemical Engineering, Nanjing University of Technology, 5 Xinmofan Road, Nanjing, 210009, P. R. China

[b]Department of Chemical and Biomolecular Engineering, National University of Singapore, 117576, Singapore

Email: wqjin@njtech.edu.cn (Prof. W Jin); gpliu@njtech.edu.cn (Dr. G. Liu)

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 (H_2, CH_4, N_2 and CO_2) 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 H_2/CO_2, resulting in selective permeation shifting from CO_2 to H_2. 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