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A systematic review of the molecular simulation of hybrid membranes for performance enhancements and contaminant removals

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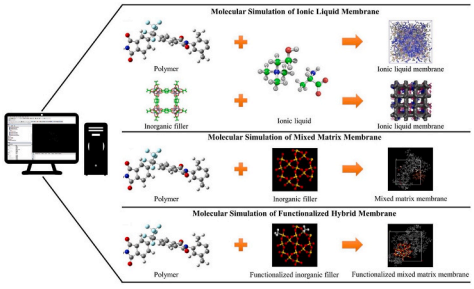
HIGHLIGHTS

- Fundamentals of molecular simulation are reviewed and related to application in hybrid membranes.
- Insight into molecular structural properties of hybrid membranes is presented.
- Simulated transport performance from published literature and mechanism of hybrid membranes are provided.
- Limitation in molecular simulation for membrane separation is discussed.
- Future outlook for molecular simulation of membrane separation is recommended.

GRAPHICAL ABSTRACT



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ABSTRACT

Number of research on molecular simulation and design has emerged recently but there is currently a lack of review to present these studies in an organized manner to highlight the advances and feasibility. This paper aims to review the development, structural, physical properties and separation performance of hybrid membranes using molecular simulation approach. The hybrid membranes under review include ionic liquid membrane, mixed matrix membrane, and functionalized hybrid membrane for understanding of the transport mechanism of molecules through the different structures. The understanding of molecular interactions, and alteration of pore sizes and transport channels at atomistic level post incorporation of different components in hybrid membranes posing impact to the selective transport of desired molecules are also covered. Incorporation of molecular simulation of hybrid membrane in related fields such as carbon dioxide (CO_2) removal, wastewater treatment,

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