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Molecular Dynamics Simulation for Membrane Separation

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Message from the Guest Editors

We are pleased to invite you to report your research findings in this Special Issue of Molecular Dynamics Simulation for Membrane Separation. Computational studies and molecular dynamics (MD) simulations have elucidated various aspects of membrane technology across diverse sub-sectors. Due to their intricate microporous structure and complex biochemical composition, separative membrane materials exhibit varying levels of complexity. Significantly, the incorporation of nanocomposite materials into membranes increases the complexity of the structure, particularly in the case of thin-film nanocomposites and porous separative nanocomposite materials. MD simulations, like other computational methodologies, aim to elucidate unresolved inquiries, shed light on regions of uncertainty, and offer plausible explanations and solutions.

This Special Issue aims to report how MD approaches could help to unravel the mystery of complex materials, how they interact with their environment, and how they physically, biologically, and chemically behave. MD could also be used for the investigation of current ongoing cases, or to predict the future of material science.





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Message from the Editor-in-Chief

You are cordially invited to contribute a research article or a comprehensive review for consideration and publication in *Membranes* (ISSN 2077-0375).

Membranes is an international, peer-reviewed open access journal of membrane technology published monthly online by MDPI. The journal covers the broad aspects of the science and technology of both biological and non-biological membranes, including membrane dynamics and the preparation and characterization of membranes and their applications in water, environment, energy, and food industries. Articles contributing to better understanding of transport processes in all types of membranes are also welcome. The scientific community and the general public have unlimited and free access to the content as soon as it is published. We would be pleased to welcome you as one of our authors.

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