

Special Issue

Membrane Design via Molecular Simulation and Artificial Intelligence

Message from the Guest Editor

We are pleased to invite you to contribute to the Special Issue "*Membrane Design via Molecular Simulation and Artificial Intelligence*" and share your valuable insights on related emerging technologies.

Hybrid *membranes* can synergize the advantageous properties of two or more components, thus presenting new possibilities in separation science that were challenging to achieve a decade before. This collection aims to illustrate the interesting advancements made in hybrid *membranes* aided by computational modeling and artificial intelligence approaches. Examples include, but are not limited to, two-dimensional material-doped polymer *membranes*, porous material-supported *membrane* layers, organic/inorganic laminated *membranes*, etc. Significant applications in separation science such as gas, ion, organic compounds, etc., are highly encouraged, and studies that utilize state-of-the-art atomistic simulations and artificial intelligence methods are welcome.

Guest Editor

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Deadline for manuscript submissions

closed (20 July 2025)



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About the Journal

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.

Editor-in-Chief

Prof. Dr. Spas D. Kolev
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