Special Issue

Molecular Dynamics Simulations in Biological Membranes

Message from the Guest Editor

Biological membranes are crucial components of living organisms, serving as selective barriers and facilitating various cellular processes. Understanding the intricate dynamics and interactions within these membranes is essential for advancing our knowledge of cellular function and dysfunction. Molecular dynamics (MD) simulations have emerged as a powerful tool for investigating the complex behavior of biological membranes at the molecular level. This Special Issue aims to showcase recent advances, novel applications, and cutting-edge research in the field of molecular dynamics simulations applied to biological membranes. We welcome contributions that highlight the role of MD simulations in elucidating the structure, function, dynamics, and interactions of membrane components, ranging from lipid bilayers to membrane proteins. The Special Issue will provide a platform for researchers to share their findings, methodologies, and insights, fostering collaboration and driving innovation in this exciting field.

Guest Editor

Prof. Dr. Jingjing Guo

Centre in Artificial Intelligence Driven Drug Discovery, Faculty of Applied Sciences, Macao Polytechnic University, Macao 999078, China

Deadline for manuscript submissions

31 October 2025

Membranes

an Open Access Journal by MDPI

Impact Factor 3.6
CiteScore 7.9
Indexed in PubMed

mdpi.com/si/241284

Membranes
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
membranes@mdpi.com

mdpi.com/journal/membranes

Membranes

an Open Access Journal by MDPI

Impact Factor 3.6
CiteScore 7.9
Indexed in PubMed

mdpi.com/journal/membranes

MDPI

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 accessjournal 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
School of Chemistry, The University of Melbourne, Melbourne, VIC 3010, Australia

Author Benefits

Open Access:

free for readers, with article processing charges (APC) paid by authors or their institutions.

High Visibility:

indexed within Scopus, SCIE (Web of Science), Ei Compendex, PubMed, PMC, CAPlus / SciFinder, Inspec, and other databases.

Journal Rank:

JCR - Q2 (Polymer Science) / CiteScore - Q1 (Chemical Engineering (miscellaneous))