

Special Issue

Use of Multi-Scale Simulation for Material Innovation

Message from the Guest Editor

We are living in a material world, designing functional material is key. In absence of validated data for materials, one therefore need to perform high throughput simulation to generate good property data to run data modeling to innovate new material in today's world of informatics. Molecular modeling based on molecular structure can be used to predict key properties to gain insight into the behavior of the materials and calculate properties that are relevant to material engineers. Macro scale simulation is in place to look into device properties, where the material properties comes from some standard database (there are very few databases with mixed material properties) as input and if unavailable it still is a guess, and with a vast new materials in practice; this is becoming a challenging task. Multi-scale simulation is therefore is an effort to link the gap between microscale to macro-scale through meso-scale. In this time with a new demand for new materials is the time to have the special issue to improve our understanding on this.

Guest Editor

Dr. Abhijit Chatterjee

BIOVIA Materials Science Principal Scientist, Dassault Systems Biovia K.K., ThinkPark Tower 21F, 2-1-1 Osaki, Shinagawa-ku, Tokyo 141-6020, Japan

Deadline for manuscript submissions

closed (31 July 2022)



International Journal of Molecular Sciences

an Open Access Journal
by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed



mdpi.com/si/90231

*International Journal of
Molecular Sciences*
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
ijms@mdpi.com

[mdpi.com/journal/
ijms](https://mdpi.com/journal/ijms)





International Journal of Molecular Sciences

an Open Access Journal
by MDPI

Impact Factor 4.9
CiteScore 9.0
Indexed in PubMed



[mdpi.com/journal/
ijms](https://mdpi.com/journal/ijms)



About the Journal

Message from the Editor-in-Chief

The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

Editor-in-Chief

Prof. Dr. Maurizio Battino

Department of Odontostomatologic and Specialized Clinical Sciences,
Sez-Biochimica, Faculty of Medicine, Università Politecnica delle
Marche, Via Ranieri 65, 60100 Ancona, Italy

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), PubMed, PMC, MEDLINE, Embase, CAPlus / SciFinder, and other databases.

Journal Rank:

JCR - Q1 (Biochemistry and Molecular Biology) / CiteScore
- Q1 (Organic Chemistry)