Special Issue

Computational Chemistry for Material Research

Message from the Guest Editors

Recent advances in computational chemistry have stimulated their application in material research, such as in the prediction of thermodynamic properties for catalysts, X-ray absorption spectroscopy (XAS), mechanical and elastic properties, and ion mobilities for batteries. Computational chemistry bridges theory and experimental insight for material research.This Special Issue aims to cover the large scale of materials and answer the questions that experiments are unable to. Fields to be covered that involve computational study include the following:

- Prediction of novel heterogeneous catalysts for HER, ORR, OER, NRR, etc.
- Prediction of novel anode and cathode materials for Li- and Na-ion batteries.
- Prediction and verification of lanthanide and transition-metal X-ray absorption spectroscopy, especially their L and M edges.
- Development of novel methodologies for the accurate prediction of semiconductor band gap energies.
- Fast algorithms for fast potential energy surface (PES) scanning.

Guest Editors

Dr. Tian Wang

Dr. Cheng Zhong

Dr. Tianyuan Zhang

Dr. Xiaohua Wang

Deadline for manuscript submissions

closed (30 November 2023)

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/si/127296

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

mdpi.com/journal/molecules

Molecules

an Open Access Journal by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed

mdpi.com/journal/molecules

About the Journal

Message from the Editor-in-Chief

As the premier open access journal dedicated to molecular chemistry, now in its 29th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts, and novel materials. Pushing the boundaries of the discipline, we invite papers on all major fields of molecular chemistry and multidisciplinary topics bridging chemistry with biology, physics, and materials science, as well as timely reviews and topical issues on cutting-edge fields in all of these areas.

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt
Institute of Pharmaceutical Biology and Phytochemistry, University of Münster, Corrensstrasse 48, D-48149 Münster, Germany

Author Benefits

High Visibility:

indexed within Scopus, SCIE (Web of Science), PubMed, MEDLINE, PMC, Reaxys, CaPlus / SciFinder, MarinLit, AGRIS, and other databases.

Journal Rank:

JCR - Q2 (Biochemistry and Molecular Biology) / CiteScore - Q1 (Organic Chemistry)

Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 16.1 days after submission; acceptance to publication is undertaken in 2.6 days (median values for papers published in this journal in the first half of 2025).

MDPI