Special Issue

Computational Studies of Novel Function Materials

Message from the Guest Editor

In recent years, there has been an explosion of new material discoveries. Such as low-dimensional materials, single-layer materials, multiple-layered materials, transition-metal dichalcogenides (TMD), and MXene. Those new rising materials have been investigated as catalysts, adsorbents, electrodes, and electrolytes. All these great developments of functional material discovery have led to a new era in material discovery. Computations have provided a strong ability to accelerate material discovery. For instance, computations for spectrum, stability exploration of new materials, electronic and optical properties, molecular dynamics, and adsorption ability have been employed for defining and analyzing a new material from a theoretical aspect. In light of the growing demand for new functional materials in various applications and the strong power of computations implemented in material discovery, we have decided to edit a Special Issue, "Computational Studies of Novel Function Materials".

Guest Editor

Dr. Shiru Lin

Division of Chemistry and Biochemistry, Texas Woman's University, Denton, TX 76204, USA

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/135123

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

MDPI

About the Journal

Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th 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 multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all 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).