



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)

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".





an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Thomas J. Schmidt

Institute of Pharmaceutical
Biology and Phytochemistry,
University of Münster,
Corrensstrasse 48, D-48149
Münster, Germany

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.

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](#), [MEDLINE](#), [PMC](#), [Reaxys](#), [CaPlus / SciFinder](#), [MarinLit](#), [AGRIS](#), and [other databases](#).

Journal Rank: JCR - Q2 (*Chemistry, Multidisciplinary*) / CiteScore - Q1 (*Chemistry (miscellaneous)*)

Contact Us

Molecules Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/molecules
molecules@mdpi.com
[X@Molecules_MDPI](#)