

Special Issue

Computational and Experimental Research on Materials for Environmental Applications

Message from the Guest Editors

The editorial board of *Molecules* (IF: 4.6, ISSN 1420-3049) invites you to submit an article or review to a Special Issue entitled "Computational and Experimental Research on Materials for Environmental Applications". This Special Issue aims to present modern interdisciplinary research that advances our understanding of material behavior and performance in environmental contexts. We welcome contributions that are purely experimental, but have a particular interest in those that integrate both experimental and computational approaches to provide comprehensive insights into material design, mechanisms, and applications. Studies on nanomaterials, heterogeneous catalysis, adsorption, environmental remediation, and pollutant removal, are vitally important for advancing our discipline. Experimental investigations that lead to real-world applications, as well as computational studies that provide predictive or mechanistic insight, are equally welcome.

Guest Editors

Dr. Sanja J. Armakovic

Dr. Stevan Armaković

Dr. Maria M. Savanović

Deadline for manuscript submissions

30 April 2026



Molecules

an Open Access Journal
by MDPI

Impact Factor 4.6
CiteScore 8.6
Indexed in PubMed



mdpi.com/si/252509

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

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