



an Open Access Journal by MDPI

Theoretical Chemistry and Computational Simulations in Nanomaterials

Guest Editors:

Dr. Dashuai Wang

1. Institute of Zhejiang University-
Quzhou, Quzhou 324000, China
2. Key Laboratory of Biomass
Chemical Engineering of Ministry
of Education, College of
Chemical and Biological
Engineering, Zhejiang University,
Hangzhou 310027, China

Dr. Xianyun Peng

1. Institute of Zhejiang University-
Quzhou, Quzhou 324000, China
2. College of Chemical and
Biological Engineering, Zhejiang
University, Hangzhou 310027,
China

Deadline for manuscript
submissions:

closed (30 May 2025)

Message from the Guest Editors

With the rapid advancement of nanoscience and nanotechnology, researchers increasingly rely on theoretical and computational approaches for the design, prediction of properties, and optimization of nanomaterials. Theoretical chemistry and computational simulations play a pivotal role in elucidating fundamental principles, in explaining experimental phenomena, and in guiding the synthesis and applications of nanomaterials. This Special Issue provides a platform for researchers to exchange ideas, showcase cutting-edge research findings, and discuss methodological developments.

This Special Issue aligns closely with the scope of the journal *Nanomaterials*, which focuses on the publication of research papers addressing both scientific and applied aspects of nanomaterials. It offers an excellent opportunity to present the latest advancements in theoretical chemistry and computational simulations within the field of nanomaterials. We welcome original research articles and reviews that cover a wide range of topics.



mdpi.com/si/184501

Special Issue



an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Eugenia Valsami-Jones

School of Geography, Earth and
Environmental Science,
University of Birmingham,
Birmingham B15 2TT, UK

Message from the Editor-in-Chief

Nanoscience and nanotechnology are exciting fields of research and development, with wide applications to electronic, optical, and magnetic devices, biology, medicine, energy, and defense. At the heart of these fields are the synthesis, characterization, modeling, and applications of new materials with lower nanometer-scale dimensions, which we call “nanomaterials”. These materials can exhibit unusual mesoscopic properties and include nanoparticles, coatings and thin films, metal-organic frameworks, membranes, nano-alloys, quantum dots, self-assemblies, 2D materials such as graphene, and nanotubes. Our journal, *Nanomaterials*, has the goal of publishing the highest quality papers on all aspects of nanomaterial science to an interdisciplinary scientific audience. All of our articles are published with rigorous refereeing and open access.

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](#), [CAPus / SciFinder](#), [Inspec](#), and [other databases](#).

Journal Rank: JCR - Q2 (Physics, Applied) / CiteScore - Q1 (General Chemical Engineering)

Contact Us

Nanomaterials Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

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

mdpi.com/journal/nanomaterials
nanomaterials@mdpi.com
[X@nano_mdpi](#)