Special Issue

First Principles Study of Two-Dimensional Materials

Message from the Guest Editor

With the innovation of high-performance computers, the computational design of materials is gaining increasing attention. Among different computational methods, first-principles calculation has rapidly developed for its accuracy and lack of dependence on empirical parameters. This method has been applied in various materials (solid, surface, 2D materials, etc.) and various properties (magnetic, catalytic, optical, etc.) can be accessed by it. However, much remains to be carried out in the first-principles community, such as the development of new theories and the design of new materials. We welcome contributions on the current trends in this field, including but not limited to the following topics:

- New theories of first-principles simulation;
- New materials designed by first-principles calculations;
- New properties investigated by first-principles calculations;
- New insights into traditional materials using first-principles calculations.

Guest Editor

Dr. Haiming Lu

College of Engineering and Applied Sciences, Nanjing University, Nanjing, China

Deadline for manuscript submissions

closed (20 September 2025)

Nanomaterials

an Open Access Journal by MDPI

Impact Factor 4.3
CiteScore 9.2
Indexed in PubMed

mdpi.com/si/228465

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

mdpi.com/journal/nanomaterials

Nanomaterials

an Open Access Journal by MDPI

Impact Factor 4.3
CiteScore 9.2
Indexed in PubMed

mdpi.com/journal/nanomaterials

About the Journal

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. We are proud of our increasing impact factor and ability to provide rapid decisions to authors.

Editor-in-Chief

Prof. Dr. Eugenia Valsami-Jones
School of Geography, Earth and Environmental Science, University of Birmingham, Birmingham B15 2TT, UK

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, CAPlus / SciFinder, Inspec, and other databases.

Journal Rank:

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

MDPI