

## 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

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### Deadline for manuscript submissions

20 September 2025



## Nanomaterials

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## 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.

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### Editor-in-Chief

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