Special Issue

First-Principle Calculation Study of Nanomaterials

Message from the Guest Editors

This Special Issue of *Nanomaterials* focuses on first-principles calculations of nanomaterials' properties and applications. This Special Issue aims to offer a timely and authoritative opportunity to present recent progress in first-principles calculations of nanomaterials and their applications. In this Special Issue, theoretical original research articles and reviews are welcome. Research areas may include (but are not limited to) the following:

- Calculating properties of nanomaterials, such as nanoparticles, coatings, and thin films, inorganic-organic hybrids and composites (i.e., MOFs), membranes, nano-alloys, quantum dots, self-assemblies, graphene, nanotubes, etc.;
- Theoretical design/optimization of new organic, inorganic, and hybrid nanomaterials;
- New theoretical methods for/approaches to nanomaterials;
- Use of ML/AI to bridge the gap between accessible DFT scales and the nanoscale;
- Characterization of mesoscopic properties;
- Modeling of mesoscopic properties and effects;
- Theoretical simulations of any application of new nanomaterials or new application of nanomaterials;
- Carbon nanotubes.

We look forward to receiving your contributions.

Guest Editors

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Deadline for manuscript submissions

closed (20 December 2023)

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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.

Editor-in-Chief

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