

## Special Issue

# First-Principles Investigations of Low-Dimensional Nanomaterials (2nd Edition)

### Message from the Guest Editors

Low-dimensional nanomaterials usually exhibit various physical and chemical properties in comparison with the three-dimensional bulk materials, mainly due to ample configurations in OD NCs, edge states in 1D NRs/NTs, and a high surface-to-volume ratio in 2D NSs; therefore, lowdimensional nanomaterials can be used in a wide range of fields. This Special Issue of Nanomaterials aims to present recent developments of low-dimensional nanomaterials in terms of first-principles investigations, covering structures, stability, magnetic characteristics, electronic features, mechanical properties, energy storage performance, sensing capability, energy conversion behavior, and the origin of their physical and chemical characteristics. For this Special Issue, we invite contributions from leading groups in this field with the objective of providing original research articles and review articles on the current state-of-the-art advances in this exciting discipline. See more information in: <https://www.mdpi.com/si/185043>

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### Guest Editors

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### Deadline for manuscript submissions

closed (8 August 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. We are proud of our increasing impact factor and ability to provide rapid decisions to authors.

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### Editor-in-Chief

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