Special Issue

Theory and Modeling of Nanostructured Materials

Message from the Guest Editors

We invite researchers from academia, industry, and research institutions to submit their original research, review articles, and perspectives on the theoretical modelling and simulation of low-dimensional systems, including quantum dots, single crystals, multicomponent or polycrystalline and layered nanoparticles, nanotubes, and nanorods. Potential topics of interest for this Special Issue include, but are not limited to:

- nanostructured materials
- nanocrystals
- layered materials
- nanotubes
- quantum dots
- Finite-Element Modelling (FEM)
- Monte Carlo (MC)
- Molecular Dynamics (MD) & Molecular Mechanics (MM)
- Ab-initio & Density Functional Theory (DFT)

We look forward to receiving your contributions. See more information in https://www.mdpi.com/si/259309

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Deadline for manuscript submissions

closed (1 May 2026)

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

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