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Advances in Computational Modeling and Simulation of Nanoscale Materials

Guest Editor:

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Deadline for manuscript submissions:
closed (31 December 2024)

Message from the Guest Editor

This Special Issue aims to consider computational materials methods for the design and discovery of nanoscale materials across diverse applications, spanning electronics, optoelectronics, energy harvesting and storage and aerospace and ranging from cryogenic to moderate to extreme environments. It encompasses quantum computing, first-principle computations and atomistic simulations, as well as meso-, macro-, and multi-scale modeling. The focus extends to the integration of artificial intelligence, machine learning, and quantum machine learning methods. Research addressing the understanding and design of multifunctional nanomaterials in dimensions like 0D, 1D, 2D, thin films, heterostructures, moiré heterostructures, and interfaces is welcome. We invite submissions across a broad spectrum of studies dedicated to leveraging computational strategies for the design and discovery of nanoscale materials.

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Editor-in-Chief

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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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