

Special Issue

Computational Modeling and Simulation for Nanomaterials, Nanotechnology, and Nanoscience

Message from the Guest Editor

Nanoscience and nanotechnology emerged in the last decades at the forefront of a wide array of research fields, due to the highly challenging and surprising properties of nanomaterials and nanosystems. When accounting for the effects of various phenomena occurring at the nanoscale, models and simulations together tend to reveal unsolved issues while enabling formidable advances that push forward the rich spectrum of technologies based on nanostructured materials. Moreover, it is clear that, for such materials, theoretical formulations and numerical solvers, dealing with mesoscopic or macroscopic descriptions, are necessary tools to enhance experiments and practical investigations. This Special Issue aims to gather the rich variety of recent research breakthroughs in the perspective described above, and it aims to cover recent advances in the study of phenomena, the manipulation of materials at different scales, the design and characterization of nanoapplications, all enabled by computational modeling and simulation of nanomaterials.

Guest Editor

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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.

Editor-in-Chief

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