Special Issue

Advances in Theoretical and Computational Physics of Low-Dimensional Materials

Message from the Guest Editor

Recent breakthroughs in nanotechnology have spurred interest in low-dimensional materials, from atomically thin semiconductors to carbon nanostructures, which exhibit unique properties different from their bulk counterparts. To rationally develop these materials, a precise understanding of complex quantum interactions and structural sensitivities is essential. Theoretical modeling and computational simulations have become vital for decoding structure–property relationships at unprecedented resolutions. This Special Issue focuses on advancing methodologies that combine physical principles with numerical techniques to interpret experiments and predict novel functionalities. Topics include theoretical and simulation approaches, prediction of structures and properties, exploration of fundamental behaviors and degradation, integrative computational-experimental studies, and design using machine learning and artificial intelligence.

Guest Editor

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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.

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