Special Issue

Computational Quantum Physics and Chemistry of Nanomaterials

Message from the Guest Editor

Nanomaterials become more and more important both in basic research and in applications. Some properties may be understood only at the level of the quantum-mechanical study of these materials. The purpose of this Special Issue is to advance our fundamental understanding of the structure and technologically important properties of nanomaterials with the help of computational quantum solid-state physics and chemistry. There is no doubt that quantum-mechanical approaches are indispensable in comprehensive studies of nanomaterials and will be more and more crucial in the future. Of course, this field is too extensive and too diverse to be described in a single volume. Nevertheless, this Special Issue should provide at least a partial snapshot of the state-of-the-art of computational quantum-mechanical studies of nanomaterials, cover some recent advances and problems, and discuss promising future directions in this field.

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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