Special Issue

Computational Approaches to Electronic Structures and Properties of Nanomaterials

Message from the Guest Editor

Nanomaterials have emerged as a revolutionary development in materials science and engineering. Their unique electronic properties at the nanoscale have opened doors to countless applications, from electronics and energy storage to catalysis and medicine. However, due to their nanoscale nature, experimental characterization can be challenging and expensive. Computational methods have become indispensable for researchers seeking to addresses these challenges and explore the electronic intricacies of nanomaterials. These methods provide a cost-effective and insightful means to predict, understand, and design electronic structures and properties at the nanoscale. This Special Issue aims to provide a platform for researchers to disseminate their findings and insights on the electronic structures and properties of nanomaterials using state-of-the-art computational methods, including, but not limited to, density functional theory (DFT), molecular dynamics (MD) simulations, and Monte Carlo simulations. We welcome submissions of original research articles and systematic reviews.

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

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