Special Issue

Advances in Molecular Simulation and Modeling of Nanomaterials

Message from the Guest Editor

The most recent advances in high-performance computing have resulted in impressive progress in the complexity of the physicochemical systems that can be described at atomistic or molecular scales. This means that the boundaries of the time and distance scales that can be dealt with using quantum calculations, classical molecular simulation techniques, or hybrid approaches are being astonishingly enhanced. This opens new perspectives for the description of nanoscale phenomena using a variety of atomistic scale theoretical approaches, yielding rigorous descriptions of the underlying physics and chemistry. In this dynamic and fast-moving scenario, contributions that describe molecular modelling descriptions of nanostructured systems are welcome in this Special Issue. Please see more details at the following link: https://www.mdpi.com/si/171456

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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