Special Issue

Machine Learning and Multi-Scale Modelling for Functional Nanomaterials

Message from the Guest Editor

Functional nanomaterials have been widely used in various fields due to their distinctive physiochemical properties. Theoretical simulations play a very important role in the development of functional nanomaterials because they can provide deep insight into the structures, properties, spectra, etc. The past few decades have witnessed rapid progress in computational power and advanced theoretical modeling algorithms. In particular, molecular dynamics (MD) simulations, first-principles calculations, multi-scale modelling and machine learning have gained ever-increasing popularity in the design and study of functional nanomaterials. This Special Issue's potential topics include, but are not limited to:

- The development of machine learning methods in physics, chemistry, materials and life science;
- Advanced numerical methods for solving multi-scale problems;
- Simulation and modelling of multi-scale systems. etc.

See more information at
https://www.mdpi.com/si/182055

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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