Special Issue

Nanomaterials Investigation by Molecular Dynamics Simulation

Message from the Guest Editor

Fast progress in the nanomaterials sciences is related to the development of computer methods: computational materials sciences. Today, more attention is being paid to a universal method for modeling the properties of nanomaterials—molecular dynamics (MD). MD simulation is a method where time evolution of an ensemble of interacting atoms is determined by integrating the equations of their motion. The interaction between objects in a system can be described by classical MD using molecular mechanics (MM) force field methods, by quantum-mechanical (QM) methods or mixed approaches containing both QM/MM. This special issue focuses on computational studies of nanomaterials based on various components using MD modeling in various areas: nanoparticles, nanolayers, nanofibers, nanotubes. MD simulations are in thin film polymeric ferroelectrics, transition metal dichalcogenides, graphene/graphene-like structures. Large-scale MD simulation and high-performance supercomputer calculations make it possible to study molecular clusters and thin films, the films deposition; quantum MD makes it possible to simulate the formation of biomacromolecules and amorphous states of materials.

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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