

Special Issue

Simulation and Modeling of Nanomaterials

Message from the Guest Editor

This Special Issue focuses on computational detailed studies (simulation, modeling, and calculations) of the structures, main properties, and peculiarities of the various nanomaterials (nanocrystals, nanoparticles, nanolayers, nanofibers, nanotubes, etc.) based on various elements, including organic and biological components, such as amino acids and peptides, etc. For many practical applications in nanoelectronics, etc., such materials as ferroelectrics and ferromagnetics, having switching parameters (polarization, magnetization), are highly requested, and simulation of dynamics and kinetics of their switching are a very important task. Another important task for these studies is also computer modeling, as well as research on the composites of these nanostructures with polymeric ferroelectrics and various graphene-like 2-dimensional structures and their properties.

Guest Editor

Dr. Vladimir S. Bystrov

Institute of Mathematical Problems of Biology RAS—The Branch of Keldysh Institute of Applied Mathematics of Russian Academy of Sciences (IMPB RAS—Branch of KIAM RAS), 142290 Pushchino, Moscow Region, Russia

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Nanomaterials
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
nanomaterials@mdpi.com

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About the Journal

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.

Editor-in-Chief

Prof. Dr. Eugenia Valsami-Jones

School of Geography, Earth and Environmental Science, University of
Birmingham, Birmingham B15 2TT, UK

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