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

Prof. Dr. Manuel M. Piñeiro
Department of Applied Physics, University of Vigo, 36310 Vigo, Spain

Deadline for manuscript submissions

closed (22 November 2023)

Nanomaterials

an Open Access Journal by MDPI

Impact Factor 4.3
CiteScore 9.2
Indexed in PubMed

mdpi.com/si/171456

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

mdpi.com/journal/nanomaterials

Nanomaterials

an Open Access Journal by MDPI

Impact Factor 4.3
CiteScore 9.2
Indexed in PubMed

mdpi.com/journal/nanomaterials

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

Editor-in-Chief

Prof. Dr. Eugenia Valsami-Jones
School of Geography, Earth and Environmental Science, University of Birmingham, Birmingham B15 2TT, UK

Author Benefits

Open Access:

free for readers, with article processing charges (APC) paid by authors or their institutions.

High Visibility:

indexed within Scopus, SCIE (Web of Science), PubMed, PMC, CAPlus / SciFinder, Inspec, and other databases.

Journal Rank:

JCR - Q2 (Physics, Applied) / CiteScore - Q1 (General Chemical Engineering)

MDPI