Special Issue

Computational Chemistry in Bionanotechnology

Message from the Guest Editor

Computational chemistry techniques range from firstprinciple approaches, such as ab initio methods and density functional theory (DFT), which are based on quantum chemistry, to semi-empirical methods, such as density functional tight binding (DFTB), which facilitate simulations using pre-fitted parameters, to molecular mechanics (MM) and molecular dynamics (MD) calculations, which are based on approximate classical potentials.

The recent combination of nanotechnology and biology has led to the development of vital systems, both in biology and in nanoengineered materials. Bionanotechnology is today an established and cuttingedge interdisciplinary research area that is located at the interface between chemistry, physics, biology, materials science, engineering, and medicine, and that finds application in numerous technological fields.

The purpose of this Special Issue, entitled "Computational Chemistry in Bionanotechnology", is to focus on the biomedical, food, agricultural, energy, and environmental fields. You can see more details at the following link: https://www.mdpi.com/si/180350

Guest Editor

Dr. Emiliano Laudadio

Department of Science and Engineering of Materials, Environment and Urban Planning, Polytechnic University of Marche, 60121 Ancona, Italy

Deadline for manuscript submissions

closed (10 March 2024)



Nanomaterials

an Open Access Journal by MDPI

Impact Factor 4.3 CiteScore 9.2 Indexed in PubMed



mdpi.com/si/180350

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



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 nanometerscale 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

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)