Special Issue

Progress in Quantum-Computer Calculations

Message from the Guest Editor

Electronic structure calculations have become an indispensable theoretical tool in physics, chemistry, and materials science. After four decades of rapid development, these calculations now allow us to study systems consisting of up to a few thousands of atoms. Further upscaling to vet bigger systems, such as those encountered in nanoparticles and other nanosystems, is all too often hindered by limited computer power of classical (super-)computers. Fortunately, there is a newly emerging class of quantum computers that should soon provide an exponentially higher computer power. Albeit promising, quantum computers are still in their infancy, and basic algorithms need to be developed. This Special Issue welcomes submissions focused primarily (but not solely) on recent developments in the broad field of quantum computers and their applications, especially software tools allowing for electronic structure calculations on quantum computers in physics, chemistry or materials science, as well as calculations on (i) either classical computer simulators of quantum processors or (ii) actual quantum computers.

Guest Editor

Dr. Martin Friák

Institute of Physics of Materials of the Czech Academy of Sciences, Brno, Czech Republic

Deadline for manuscript submissions

closed (30 June 2022)



Nanomaterials

an Open Access Journal by MDPI

Impact Factor 4.3
CiteScore 9.2
Indexed in PubMed



mdpi.com/si/69682

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



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)

