



an Open Access Journal by MDPI

Quantum Computing and Quantum Machine Learning for Nanomaterials Design and Discovery

Guest Editors:

Dr. Ali Ramazani

Department of Mechanical Engineering, Massachusetts Institute of Technology (MIT), Cambridge, MA, USA

Dr. Yuhua Duan

National Energy Technology Laboratory, United States Department of Energy, 626 Cochran Mill Road, Pittsburgh, PA 15236, USA

Prof. Dr. Veera Sundararaghavan

Department of Aerospace Engineering, University of Michigan, 1221 Beal Avenue, Ann Arbor, MI 48109-2102, USA

Deadline for manuscript submissions:

closed (24 July 2023)

Message from the Guest Editors

Quantum computing and simulations play a central role in quantum information science (QIS), and several quantum computers have already been used to model physical, electronic, chemical, vibrational, and optical properties of atoms, molecules, and materials.

The current Special Issue covers all manuscripts utilizing quantum computing simulations and algorithms, and quantum machine learning to understand, design and discover novel and high-performance nanomaterials, quantum materials, and quantum devices. We welcome the submission of all studies dealing with quantum computing and quantum machine learning in materials design and discovery. In addition, it is understood that quantum computers have limitations with respect to qubit availability and noise, therefore, papers that explore and benchmark how the current quantum algorithms can perform under these limitations or that propose new theoretical methods that may overcome these limitations considering hardware improvements are also welcome.



mdpi.com/si/148990

Special Issue



an Open Access Journal by MDPI

Editor-in-Chief

Prof. Dr. Shirley Chiang

Department of Physics, University
of California Davis, One Shields
Avenue, Davis, CA 95616-5270,
USA

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.

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 (*Chemistry, Multidisciplinary*) / CiteScore - Q1 (General Chemical Engineering)

Contact Us

Nanomaterials Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/nanomaterials
nanomaterials@mdpi.com
[X@nano_mdpi](https://x.com/nano_mdpi)