

## Special Issue

# Mathematical and Computational Modeling for Nanohybrids

### Message from the Guest Editor

The Special Issue, entitled “Mathematical and Computational Modelling for Nanohybrids”, welcomes the numerical research of nanohybrids by means of computation, numerical analyses, modeling, and the interplay of modeling and computational mathematics. Nanohybrids are materials with organic and inorganic components that are linked together at the nanometer scale. All numerical investigations are encouraged, including first-principles calculations, molecular dynamics simulations, Monte Carlo simulations, tight-banding, phase fields, finite element methods, multiscale modeling, and other mathematical and computational models. This Special Issue will especially focus on the studies of various properties (structural, mechanical, electrical, thermal, optical, acoustic, chemical, etc.) of nanohybrids for diverse applications in energy, catalysis, electronics, optoelectronics, advanced functionals, and so on. Advanced algorithms and methods for nanohybrids from all disciplines are also desirable.

### Guest Editor

Dr. Qing Peng

Physics Department, King Fahd University of Petroleum and Minerals,  
Dhahran 31261, Saudi Arabia

### Deadline for manuscript submissions

closed (10 January 2024)



## Nanomaterials

---

an Open Access Journal  
by MDPI

---

Impact Factor 4.3  
CiteScore 9.2  
Indexed in PubMed



[mdpi.com/si/124231](https://mdpi.com/si/124231)

*Nanomaterials*  
Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland  
Tel: +41 61 683 77 34  
[nanomaterials@mdpi.com](mailto:nanomaterials@mdpi.com)

[mdpi.com/journal/  
nanomaterials](https://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](https://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.

---

### 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, CAPIus / SciFinder, Inspec, and other databases.

#### Journal Rank:

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