

## Special Issue

# Theoretical and Computational Study and Modelling on Novel Nanostructures

### Message from the Guest Editors

The improved requirements in manufacturing nanotechnology have favoured the development of enhanced nanostructures with high mechanical properties, permeability, and electrical conductivity primarily made of carbon-based materials, as carbon nanotubes (CNTs), graphene sheets, or nanoplatelets. The complicated nature of these structural systems requires a proper investigation of their fundamental properties on a small scale, especially from a theoretical and computational standpoint. Advanced theories and high-performance computational models for the statics or dynamics of nano-systems are welcomed, as well as those concerning the development of enhanced non-local damage and fracturing problems which are able to capture the formation and propagation of the internal cracks related to the heterogeneity of complex materials and interfaces.

---

### Guest Editors

Dr. Rossana Dimitri

Dr. Francesco Tornabene

Dr. Matteo Viscoti

---

### Deadline for manuscript submissions

closed (30 April 2025)



## Nanomaterials

---

an Open Access Journal  
by MDPI

---

Impact Factor 4.3  
CiteScore 9.2  
Indexed in PubMed



[mdpi.com/si/214296](https://mdpi.com/si/214296)

*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)