

## Special Issue

# Development and Research on Theoretical Chemistry in Materials

### Message from the Guest Editor

- This Special Issue is intended to act as a contributor to this discussion and to future developments on this theme. We are pleased to invite you to present cutting-edge research at the intersection of theoretical chemistry and materials science in all classes of materials, highlighting how theoretical and computational approaches are revolutionizing our understanding of material properties, design, and applications. This Special Issue will cover a wide range of topics, including quantum chemical calculations (density functional theory and ab initio methods), molecular dynamics simulations, and machine learning techniques applied to materials research.
- Full papers, communications, and reviews are all welcome. Research areas may include (but are not limited to) the following: novel theoretical methods, predictive modeling of material properties, and computational studies that guide experimental work in materials development.

### Guest Editor

Dr. Alberto Gutiérrez

Department of Chemistry, University of Burgos, 09001 Burgos, Spain

### Deadline for manuscript submissions

20 February 2026



## Materials

an Open Access Journal  
by MDPI

Impact Factor 3.2  
CiteScore 6.4  
Indexed in PubMed



[mdpi.com/si/220023](https://mdpi.com/si/220023)

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

[mdpi.com/journal/  
materials](https://mdpi.com/journal/materials)





# Materials

---

an Open Access Journal  
by MDPI

---

Impact Factor 3.2  
CiteScore 6.4  
Indexed in PubMed



[mdpi.com/journal/  
materials](https://mdpi.com/journal/materials)



## About the Journal

### Message from the Editor-in-Chief

*Materials* (ISSN 1996-1944) was launched in 2008. The journal covers twenty-five comprehensive topics: biomaterials, energy materials, advanced composites, advanced materials characterization, porous materials, manufacturing processes and systems, advanced nanomaterials and nanotechnology, smart materials, thin films and interfaces, catalytic materials, carbon materials, materials chemistry, materials physics, optics and photonics, corrosion, construction and building materials, materials simulation and design, electronic materials, advanced and functional ceramics and glasses, metals and alloys, soft matter, polymeric materials, quantum materials, mechanics of materials, green materials, general. *Materials* provides a unique opportunity to contribute high quality articles and to take advantage of its large readership.

---

### Editor-in-Chief

Prof. Dr. Maryam Tabrizian

1. Department of Biomedical Engineering, Faculty of Medicine and Health Sciences, McGill University, Montreal, QC H3A 2B6, Canada
2. Faculty of Dentistry and Oral Health Sciences, McGill University, 3640 Rue University, Montreal, QC H3A 0C7, Canada

---

### 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, Ei Compendex, CaPlus / SciFinder, Inspec, Astrophysics Data System, and other databases.

#### Journal Rank:

JCR - Q2 (Metallurgy and Metallurgical Engineering) /  
CiteScore - Q1 (Condensed Matter Physics)