

Special Issue

Theoretical Calculation and Simulation of Energy Materials

Message from the Guest Editor

This Special Issue aims to collect new advances in theoretical investigations on novel energy materials. We encourage the report of supercomputing applications in design and performance prediction on materials for various applications toward energy storage as well as energy conversion, including sensors, supercapacitors, lithium-ion batteries, and so on. Both bulk materials and low-dimensional materials are of interest in this collection. The content may cover electronic structures, microstructural evolution, defect formation and growth, and their influence on physical properties. Discoveries in both new materials and new development in computational methodology and physical models can make significant contributions.

Guest Editor

Prof. Dr. Shiyu Du

Engineering Laboratory of Advanced Energy Materials, Ningbo Institute of Materials Technology & Engineering, Chinese Academy of Sciences, Ningbo 315201, China

Deadline for manuscript submissions

closed (10 August 2024)



Materials

an Open Access Journal
by MDPI

Impact Factor 3.2
CiteScore 6.4
Indexed in PubMed



mdpi.com/si/144868

Materials
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
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 Editorial Board

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.

Editors-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

Prof. Dr. Yuguang Ma

State Key Laboratory of Luminescent Materials and Devices, South China University of Technology, Guangzhou 510640, China

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)