

Special Issue

Computational Materials Design for Renewable Energy Applications

Message from the Guest Editor

This Special Issue aims to consider computational materials methods to design nanomaterials for clean and efficient energy conversion and storage. It covers first-principles computations, atomistic simulations, and meso-, macro-, and multi-scale algorithms to understand and design multifunctional nanomaterials, heterostructures, and interfaces. The application must focus on sustainable energy such as photovoltaics, photo- and electrochemistry, CO₂ capture and conversion, solar fuels, thermoelectrics, batteries, and ultra-low power electronics. Our Special Issue welcomes all submissions from all studies dealing with computational approaches to energy materials.

Guest Editor

Dr. Ali Ramazani

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

Deadline for manuscript submissions

closed (31 December 2019)



Nanomaterials

an Open Access Journal
by MDPI

Impact Factor 4.3
CiteScore 9.2
Indexed in PubMed



mdpi.com/si/13189

Nanomaterials
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
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. We are proud of our increasing impact factor and ability to provide rapid decisions to authors.

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)