Special Issue

Modeling and Simulations of Nanoporous Materials: Design and Function

Message from the Guest Editor

Nanoporous materials are now widespread in the chemical industry and in biomedical devices. Rapid progress in computational power and modeling techniques has enabled the physics- and data-driven discovery of new material structures and the optimization of their functions. This Special Issue presents recent advances in the fundamentals, methodology and applications of molecular simulations for the computational design of nanoporous materials and their applications. We welcome submissions on but not limited to:

- simulation design of microporous solids;
- amorphous carbons and silicas with tailored pore-size distributions;
- data-driven approaches to nanomaterials design;
- tailoring nanoporous materials to particular applications;
- exploration of chemical space in pursuit of new porous structures, such as new zeolites, MOFs, etc;
- traditional simulations of adsorption, separation and transport in nanopores.

Guest Editor

Dr. Aleksey M. Vishnyakov
Department of Physics, Moscow State University, Kolmogorov st, 1 b. 2, Moscow 119234, Russia

Deadline for manuscript submissions

closed (20 November 2023)

Materials

an Open Access Journal by MDPI

Impact Factor 3.2
CiteScore 6.4
Indexed in PubMed

mdpi.com/si/115201

Materials
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
materials@mdpi.com

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

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)