Special Issue

Advances in Density Functional Theory (DFT) Studies of Solids (Second Volume)

Message from the Guest Editor

The aim of this Special Issue is to collect recent advances in the theoretical study of crystalline materials using first principles calculations. The DFT computations play a significant role in the analysis of a wide range of properties such as structural, electronical, optical, mechanical, vibrational, etc. In turn, a comprehensive understanding of the characteristics of materials is necessary to improve their properties. The use of DFT calculations makes it possible to significantly simplify the interpretation of experimental data, and it is clear that complex research should be carried out using both experimental and theoretical approaches, regardless of the scale of the experiment. Thus, it is no doubt that the density functional theory method is one of the most used in materials science. Keywords

- DFT calculations
- solids
- electronic structure
- electronic density of states
- structural properties
- optical properties
- vibrational properties
- magnetic properties
- bulk materials
- 2D materials

Guest Editor

Dr. Aleksandr Oreshonkov

Laboratory of Molecular Spectroscopy, Kirensky Institute of Physics, Federal Research Center KSC SB RAS, 660036 Krasnoyarsk, Russia

Deadline for manuscript submissions

closed (20 April 2025)

Materials

an Open Access Journal by MDPI

Impact Factor 3.2
CiteScore 6.4
Indexed in PubMed

mdpi.com/si/115866

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)