materials

an Open Access Journal by MDPI

IMPACT FACTOR 3.2

Indexed in: PubMed

CITESCORE 6.4

Density Functional Theory (DFT) Calculation of Materials Properties

Guest Editors:

Dr. Alessandro Ponti
Istituto di Scienze e Tecnologie Chimiche "Giulio Natta" - SCITEC, Consiglio Nazionale delle Ricerche, via C. Golgi 19, 20133 Milano, Italy

Prof. Dr. Davide Ceresoli
CNR-SCITEC, via Golgi 19, 20133 Milano, Italy

Deadline for manuscript submissions:
closed (31 December 2018)

Message from the Guest Editors

Recent years have seen an astonishing development in the field of DFT (density functional theory) calculation of the structure and properties of crystalline materials. There are several reasons underlying the present successful application of DFT to materials science: Faster and faster computers, software improvements (in capability, accuracy and user-friendliness), and theory advancement. Based on these three pillars, computing scientists are now able to describe and understand the properties and performance of real (i.e., already-synthesized) materials and to explore the immense realm of the virtual (i.e., not-yet-synthesized) materials in their quest for the best material ever. Indeed, high-throughput techniques for the search of new crystal structures and the screening of band structure traits have become very popular in the field of computational materials science.

For further reading, please follow the link to the Special Issue Website at:

http://www.mdpi.com/si/materials/density_functional_theory

Dr. Alessandro Ponti
Dr. Davide Ceresoli
Guest Editors

materials

IMPACT FACTOR 3.2 | Indexed in: PubMed | CITESCORE 6.4

an Open Access Journal by MDPI

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

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.

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)

Contact Us

Materials Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/materials
materials@mdpi.com
𝕏@Materials_Mdpi