Special Issue

Ab Initio Modeling of 2D Semiconductors and Semimetals

Message from the Guest Editor

Two-dimensional materials (2D) have been studied very intensively in recent years due to their extraordinary physical properties. Based on graphene-like monolayers, van der Waals systems may form countless multilayer structures. Their electronic properties depend on the number of 2D atomic layers and are different from those characteristic of bulk materials. In particular, the van der Waals engineering of heterostructures enables the design of novel systems with complex electronic structures. Ab initio calculations are widely used to predict band structures of 2D materials, with special attention paid to band gaps and topologically nontrivial states. Various physical properties may be studied with the density functional theory (DFT) calculations, e.g., equilibrium structural parameters, mechanical and thermodynamical stability, etc. Additional theoretical methods may be employed in investigations of more com-plex phenomena, e.g., excitonic states and transport properties (thermoelectric effect). The proposed Special Issue is to publish a set of original papers based on ab initio calculations of various properties of 2D semiconductor and semimetallic materials.

Guest Editor

Dr. Maciej J. Winiarski

Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Okólna 2, Wrocław, Poland

Deadline for manuscript submissions

20 November 2025

Materials

an Open Access Journal by MDPI

Impact Factor 3.2
CiteScore 6.4
Indexed in PubMed

mdpi.com/si/233719

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

MDPI

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)