

## Special Issue

# First-Principles Calculations of 2D Magnetic Materials

### Message from the Guest Editors

Spintronics, which uses the electron's spin for information processing, is considered one of the most promising information technologies. Among various functional spintronics materials, two-dimensional (2D) intrinsic ferromagnetic (FM) materials, including semiconductors and half-metals, integrating low dimensionality, ferromagnetism, high integration density, and magnetic anisotropy, have been considered ideal candidates for pure spin generation, injection, and transport in high-integration-density spintronic devices. Among them, the family of atomically thin 2D magnetic materials has been quickly expanding following the discovery of graphene, such as CrI<sub>3</sub>, Cr<sub>2</sub>Ge<sub>2</sub>Te<sub>6</sub>, VS<sub>2</sub>, and other Van der Waals magnetic materials, thus opening up a vast field of low-dimensional magnetism. Some of the foreseen topics to be treated in the Special Issue will be:

- Discovery of 2D magnetic materials;
- Heterostructures combining 2D magnetic materials with other materials;
- Defect modulated magnetism in 2D and layered materials;
- Optical/electronic properties and novel perspectives;
- First-principles characterization;
- Computational methods in the field of magnetism.

### Guest Editors

Dr. He Huang

Beijing Advanced Innovation Center for Materials Genome Engineering,  
School of Materials Science and Engineering, University of Science and  
Technology Beijing, Beijing 100083, China

Dr. Gang Tang

School of Interdisciplinary Science, Beijing Institute of Technology,  
Beijing, China

### Deadline for manuscript submissions

closed (10 April 2023)



## Materials

an Open Access Journal  
by MDPI

Impact Factor 3.2  
CiteScore 6.4  
Indexed in PubMed



[mdpi.com/si/134980](https://mdpi.com/si/134980)

*Materials*  
Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland  
Tel: +41 61 683 77 34  
[materials@mdpi.com](mailto:materials@mdpi.com)

[mdpi.com/journal/  
materials](https://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](https://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)