



## Atomistic Modelling and Simulation of Structural and Phase Stability in Metals and Alloys

Guest Editor:

**Dr. Pavel Korzhavii**

Department of Materials Science  
and Engineering, KTH – Royal  
Institute of Technology, SE-100  
44 Stockholm, Sweden

Deadline for manuscript  
submissions:

**closed (31 October 2020)**

### Message from the Guest Editor

The theory and methodology of atomistic modeling have recently advanced to a level where such calculations can predict the variations of physical properties of condensed matter phases with temperature, pressure, and chemical composition, starting from first principles of quantum mechanics.

The aim of this Special Issue is to present the state-of-the-art of the rapidly growing field of first-principles based atomistic modelling of the thermodynamic properties of metallic alloys. Original research papers and critical reviews are welcome, focusing on the following main topics: (i) First-principles modelling of free energy and related thermophysical properties of alloy phases; (ii) advanced approaches to atomistic modelling of multicomponent alloys (steels, superalloys, high-entropy alloys); (iii) description of vibrational, electronic/magnetic, and configurational disorder in metals and alloys at finite temperatures; (iv) modern theories of electronic factor in phase stability of metallic alloys; and (v) technologies and challenges of multiscale modeling: Data representation, storage, and mining.





an Open Access Journal by MDPI

## Editors-in-Chief

### Prof. Dr. Hugo F. Lopez

Department of Materials Science and Engineering, College of Engineering & Applied Science, University of Wisconsin-Milwaukee, 3200 N. Cramer Street, Milwaukee, WI 53211, USA

### Prof. Dr. Yong Zhang

Beijing Advanced Innovation Center of Materials Genome Engineering, State Key Laboratory for Advanced Metals and Materials, University of Science and Technology Beijing, 30 Xueyuan Road, Beijing 100083, China

## Message from the Editorial Board

Metallic materials play a vital role in the economic life of modern societies; contributions are sought on fresh developments that enhance our understanding of the fundamental aspects related to the relationships between processing, properties and microstructure – disciplines in the metallurgical field ranging from processing, mechanical behavior, phase transitions and microstructural evolution, nanostructures, as well as unique metallic properties – inspire general and scholarly interest among the scientific community.

## 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), Inspec, CAPlus / SciFinder, and other databases.

**Journal Rank:** JCR - Q2 (*Metallurgy and Metallurgical Engineering*) / CiteScore - Q1 (Metals and Alloys)

## Contact Us

---

Metals Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland

Tel: +41 61 683 77 34  
[www.mdpi.com](http://www.mdpi.com)

[mdpi.com/journal/metals](http://mdpi.com/journal/metals)  
[metals@mdpi.com](mailto:metals@mdpi.com)  
[X@Metals\\_MDPI](https://twitter.com/Metals_MDPI)