Special Issue

Molecular Dynamics Study of Metal Alloys

Message from the Guest Editors

The optimization of metal alloy compositions is a practical route to achieve the target strength and stiffness of materials for engineering applications. Molecular dynamics (MD) simulations with an appropriate choice of interatomic potential can provide unprecedented details of the behavior of materials. elucidate the dynamics of defects, and fracture mechanisms. The recent advances in the development of interatomic potentials and high-performance computing facilities enabled in silico discovery of new alloy compositions with extraordinary mechanical properties and unraveling the structure-property relationships to guide their experimental synthesis. In particular, the design of the emerging class of materials such as shape memory alloys (SMA) and high-entropy alloys (HEA) can heavily benefit from the a priori prediction of the strength and related properties from the MD simulations. The Special Issue is focused on "Molecular Dynamics Study of Metal Alloys", with the aim to collect original research articles and scientific reviews highlighting cutting-edge and innovative scientific advancements and future directions in this field.

Guest Editors

Prof. Dr. Md Mahbubul Islam

Department of Mechanical Engineering, Wayne State University, Detroit, MI 48202, USA

Prof. Dr. Aniruddh Vashisth

Department of Mechanical Engineering, University of Washington, Seattle, WA 98195, USA

Deadline for manuscript submissions

closed (30 December 2021)



Metals

an Open Access Journal by MDPI

Impact Factor 2.5 CiteScore 5.3



mdpi.com/si/76893

Metals
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
metals@mdpi.com

mdpi.com/journal/ metals





Metals

an Open Access Journal by MDPI

Impact Factor 2.5 CiteScore 5.3



About the Journal

Message from the Editor-in-Chief

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.

Editor-in-Chief

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

Author Benefits

High Visibility:

indexed within Scopus, SCIE (Web of Science), Inspec, Ei Compendex, CAPlus / SciFinder, and other databases.

Journal Rank:

JCR - Q2 (Metallurgy and Metallurgical Engineering) / CiteScore - Q1 (Metals and Alloys)

Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 18 days after submission; acceptance to publication is undertaken in 2.6 days (median values for papers published in this journal in the first half of 2025).

