

Special Issue

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

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.

Guest Editor

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Deadline for manuscript submissions

closed (31 October 2020)



Metals

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About the Journal

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.

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