Special Issue

Thermodynamic Modeling of Phase Equilibrium in Metallic Materials

Message from the Guest Editor

The choice of materials has become a key element in the environmentally friendly industry. Sustainability through materials allows for a better use of energy, improved efficiency, and lower costs. The development of green technologies and sustainable materials plays an important role in addressing the climate change challenge. In order to design alloys, computer simulation of phase diagrams has major importance. CALPHAD methodology is used to predict thermodynamic, kinetic, and other properties of multicomponent material systems. New emerging methods such as artificial intelligence have been recently introduced to simulate phase diagrams. This Special Issue aims to address the latest research devoted to the thermodynamic modeling of phase equilibrium and other properties in metallic materials, especially for sustainable materials for energy (e.g., nuclear), automotive, aerospace, and other applications.

- thermodynamic modeling
- phase diagrams
- solidification
- alloying design
- CALPHAD
- Gibbs energy function
- artificial intelligence
- corrosion

Guest Editor

Prof. Dr. Ludovic Samek

Faculty for Engineering and Environmental Sciences, University of Applied Sciences Upper Austria, Stelzhamerstrasse 23, Office O2-001, 2nd Floor, A-4600 Wels, Austria

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

mdpi.com/journal/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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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

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