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Data-Driven Approaches in Modeling of Intermetallics

Guest Editor:

Dr. Anil Kunwar
Faculty of Mechanical Engineering, Silesian University of Technology, Konarskiego 18A, 44-100 Gliwice, Poland

Deadline for manuscript submissions:
closed (30 April 2022)

Message from the Guest Editor

Intermetallic compounds (IMCs) find potential applications in broad areas. The uncertainty associated in IMCs structure/composition prediction from arbitrary set of combining base metals, and opacity of adjacent metallic microstructures are the major challenges related to IMC study with experimental approach (1st paradigm) and/or theoretical approach (2nd paradigm) alone .

Computational Science and big data-driven Science can remarkably enable the robust design and discovery of intermetallic compounds. Machine learning models introduce the multivariate modeling of intermetallic compounds and therefore assist in elimination of all the barriers associated with the design and discovery of IMC materials.
Therefore it is necessary to design the data-driven approaches in modeling of intermetallics. This Special Issue is aimed at recent advances in data-driven methods as applied to intermetallics, including the aspects of machine learning and/or CALPHAD-based phase field models.

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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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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
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