Special Issue

Computational Thermodynamics

Message from the Guest Editor

The aim of this Special Issue is to encourage scholars to submit original research articles addressing one or more of the following topics: (1) Development of the next generation of CALPHAD-based thermodynamic databases: (2) estimation, modelling, and experimental determination of thermophysical properties of materials; (3) investigation of chemical reactions at interfaces and/or diffusion calculations, e.g., of metal melt/ceramic systems; (4) phase field modelling and calculations, e.g., chemical thermodynamics or in combination with continuum mechanics; and (5) simulation of 3D printing processes in combination with chemical thermodynamics. Studies focusing on similar topics and multi-disciplinary works are welcome. This Special Issue will present an overview of the actual developments in CALPHAD-based thermodynamic databases and it will show current trends of their applications.

Guest Editor

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Deadline for manuscript submissions

closed (30 September 2022)



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Editor-in-Chief

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