Computational Thermodynamics

Guest Editor:

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Deadline for manuscript submissions:
closed (30 September 2022)

Message from the Guest Editor

Dear Colleagues,

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.

Dr. Tilo Zienert
Guest Editor

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Special Issue

Editor-in-Chief

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Message from the Editor-in-Chief

The concept of entropy is traditionally a quantity in physics that has to do with temperature. However, it is now clear that entropy is deeply related to information theory and the process of inference. As such, entropic techniques have found broad application in the sciences.

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