Special Issue

Computational Thermodynamics and Its Applications

Message from the Guest Editor

Computational thermodynamics plays a crucial role in integrating phase diagrams and the thermochemistry of multi-component multi-phase systems. The Special Issue invites contributions on various aspects of computational thermodynamics and kinetics:

- Advanced applications of classical approaches, such as complex equilibrium calculations and/or multi-component phase diagrams.
- Exploring methodologies beyond complex equilibria, such as the utilization of the method of local equilibria interconnected with material streams and the incorporation of empirical methods to account for kinetic inhibitions.
- Modelling materials properties based on Gibbs-energy models for phase internal or multi-phase compositions, encompassing viscosities, densities, and surface tensions of melts.
- Establishing links between classical thermodynamic calculations and kinetic data, involving transport phenomena and reaction kinetics.
- Advancements in the generation of Gibbs energy data, including novel approaches to Calphad assessments and the development of ab-initio based Gibbs-energy datasets for elements, complex stoichiometric compounds, and solid solutions.

Guest Editor

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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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Editor-in-Chief

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