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 multicomponent 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 Gibbsenergy 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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Deadline for manuscript submissions

closed (31 August 2025)



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Editor-in-Chief

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