Thermodynamics: Modeling and Simulation

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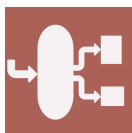Deadline for manuscript submissions:
closed (30 March 2022)

Message from the Guest Editors

In this Special Issue, "Thermodynamics: Simulation and Modeling", we highlight and celebrate the latest developments in thermodynamics research. Topics include but are not limited to the following:

- Thermodynamic models for process modeling, simulation, optimization, and control: equations of state, excess Gibbs free energy models, and related methods;
- Property prediction for early stage process development and design: molecular simulation, electronic structure calculations, and group-contribution methods;
- Molecular thermodynamics for process intensification.

We welcome contributions in the form of full-length articles, short communications, and reviews.

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Special Issue

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Message from the Editor-in-Chief

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