Special Issue

Phase Equilibrium in Chemical Processes: Experiments and Modeling

Message from the Guest Editor

We aim to present advances in experimental methods, theoretical approaches, and molecular dynamics simulations concerning vapor (or air)–liquid, liquid–liquid, solid–fluid, or multiphase systems which report new measuring techniques, experimental data, or modeling for different applications. Topics include, but are not limited to, the following:

- Phase equilibria, solvation, transport, and thermophysical properties of matters including solids, aqueous salts, or hydrates
- Extraction and separation using different solvents or mixture of solvents
- Experimental polymorphic crystallization and solid–liquid equilibria of chemicals and pharmaceuticals
- Thermodynamics of aqueous or non-aqueous mixtures
- MD and Monte Carlo simulations of macromolecules, electrolytes for battery applications, nanoconfined water, or interactions in the presence of H2 or supercritical CO2
- QM/MM calculations for the conformers, adsorption, solubility or binding energy, structural dynamics, and flexibility
- CALPHAD for thermodynamic, kinetic, and other properties of multicomponent systems using gE, cubic, and advanced EoS models

Guest Editor

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Deadline for manuscript submissions

25 December 2025

Processes

an Open Access Journal by MDPI

Impact Factor 2.8
CiteScore 5.5

mdpi.com/si/201473

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