

SUBMIT AN ABSTRACT FOR THE FOLLOWING SYMPOSIUM

DATA-DRIVEN AND COMPUTATIONAL MATERIALS DESIGN

Computational Thermodynamics and Kinetics

The annual Computational Thermodynamics and Kinetics (CTK) Symposium, celebrating in 2026 its 25th anniversary, showcases cutting-edge advances in computational methods to deepen our understanding of the thermodynamic and kinetic behavior and properties of both structural and functional materials. The symposium scope spans a broad range of scales, methods (e.g. electronic structure theory, density functional theory, ab initio, molecular dynamics, (kinetic) Monte Carlo, phase-field, CALPHAD, etc.) and applications in a wide range of materials (e.g. metals, alloys, semiconductors, composites, and more), enabling transformative insights into the stability, synthesis, processing, and performance of materials.

Topics of interest include but are not limited to:

- Innovative computational approaches and workflows for accelerating materials discovery and design;
- Prediction of materials properties (mechanics, chemistry, electronic, transport, magnetism, etc.);
- · Computational models of phase prediction, equilibria, stability, and transformations;
- Defects and defect phases prediction, equilibria, nucleation, growth, stability and transformations;
- Effect of external and internal constraints (elastic, plastic, electric, magnetic, vibrational/entropic, etc.) on the stability, microstructure, and properties of materials;
- Alloy design, microstructure control, multi-phase/multicomponent systems;
- · Computational modeling of rare events, systems out of equilibrium, and materials at extremes;

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