Computational Thermodynamics and Kinetics

The ability to compute thermodynamic and kinetic properties is rapidly transforming the field of materials science and engineering. Since 2001 this ongoing TMS symposium has highlighted advances in the tools and applications of computational thermodynamics and kinetics (CT&K), covering from the atomic to macroscale, and including applications to materials design, synthesis, processing and service. This year we continue to welcome submissions relating to novel developments and applications of CT&K methods as well as the use of established CT&K methods to explore new phenomena and materials. We also encourage submissions that help grow the ability of CT&K to impact the materials industry. These might include, but are not limited to, new understanding, new tools to design, develop, and optimize materials, and computational approaches to guide materials synthesis and control materials degradation.

Topics include:

- Molecular and mesoscale computations of thermodynamic, diffusion, and defect properties of materials, including both structural and functional materials
- Advances in computational tools for thermodynamic and kinetic assessments and predictions.
- Thermodynamics and kinetics for materials discovery, design, and synthesis

Organizers include:

Dane Morgan, University of Wisconsin - Madison (USA)
Shawn Coleman, U.S. Army Research Laboratory (USA)
Xiang-Yang (Ben) Liu, Los Alamos National Laboratory (USA)
Chris Wolverton, Northwestern University (USA)