TMS2016
145th Annual Meeting & Exhibition

FEBRUARY 14-18 DOWNTOWN NASHVILLE, TENNESSEE MUSIC CITY CENTER

Connecting the Global Minerals, Metals, and Materials Community.

Computational Methods for Spatio-temporal Scale-bridging: from Atomistics to Mesoscale

When linking structures to properties, one often needs to span disparate time and length-scales, from atomistics (lattice vibrations, lattice constant) up to the mesoscale (diffusive time, microstructure), and beyond. This poses a considerable challenge to conventional, single-scale, simulation techniques. For example, molecular dynamics can access microseconds on millions of atoms, while phase field models, by construction, operate at length scales where atomistic effects are averaged out. Bridging such gaps while preserving and upscaling the relevant physics is a pressing challenge in computational materials science, one whose solution requires the introduction of novel computational paradigms that span multiple time and length-scales. This symposium will provide a forum to address the challenges pertaining to multiscale materials modeling and scale-bridging.

Topics of interest include:

- **Bridging time scales:** such as accelerated molecular dynamics, adaptive kinetic Monte Carlo, acceleration techniques for ab initio molecular dynamics, and methods for computational kinetics
- **Bridging length scales**: such as atomistic/continuum coupling, quasi-continuum methods, large-scale/linear-scaling DFT and tight-binding, and adaptive resolution methods
- **Bridging physics**: approaches involving concurrent/sequential multi-physics coupling, frameworks embedding different scale physics (e.g., DFT into empirical potentials)
- **Novel strategies coupling atomistic and mesoscale approaches**: such as phase-field crystals, general coarse-graining/upscaling strategies, and parameter estimation from coarse-graining
- **Computational/algorithmic aspects of scale-bridging and benchmark studies**: Contributions addressing the development of scale-bridging techniques and/or the application of these techniques to specific materials research problems

Organizers include:

Danny Perez, Los Alamos National Laboratory (USA)
Dallas Trinkle, University of Illinois Urbana-Champaign (USA)
Maryam Ghazisaeidi, The Ohio State University (USA)
Srujan Rokkam, Advanced Cooling Technologies, Inc. (USA)

Learn More at www.tms.org/TMS2016

Join us at TMS2016 in Downtown Nashville, Tennessee, February 14-18!