Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A1]Symposium A-1

Chair: Anton Van der Ven(University of California Santa Barbara, United States of America)
Mon. Oct 29, 2018 1:30 PM - 3:00 PM Room6

[SY-A1]Atomistic to continuum: coarse-graining in and out of equilibrium

Invited

○Celia Reina[1], Xiaoguai Li[1], Peter Embacher[2], Nicolas Dirr[2], Johannes Zimmer[3] (1.University of Pennsylvania, United States of America, 2.Cardiff University, UK, 3.University of Bath, UK)

We will describe various spatio-temporal coarse-graining procedures to understand the thermodynamic behavior and evolution of general atomistic/particle models. We will first revisit the equilibrium setting, providing further insights into the thermodynamic potentials and the interplay between temperature and the mechanical behavior. Then, we will move to the non-equilibrium setting, where we will discuss how to compute macroscopic dissipative evolutions, in particular parameters. In all cases, the results will be validated with full resolution particle simulations.