Symposium | A. Advances in Materials Theory for Multiscale Modeling

[SY-A2] Symposium A-2

Chair: Kenjiro Sugio(Hiroshima Univ., Japan)

2018年10月29日(月) 15:45 ～ 17:30 Room6

[SY-A2]Bridging the chasm between phenomenological theories and electronic structure

Invited

○Anton Van der Ven (University of California Santa Barbara, United States of America)

The first-principles prediction of non-equilibrium materials processes remains a major challenge. The evolution of a solid out of equilibrium is affected by intrinsic thermodynamic, mechanical and kinetic properties that are often difficult if not impossible to measure accurately in isolation. Nevertheless, there are many successful phenomenological theories of phase transformations and microstructure evolution that have been formulated in terms of thermodynamic free energies and kinetic transport coefficients. One approach to treating non-equilibrium materials processes from first principles, therefore, is to predict intrinsic thermodynamic, kinetic and mechanical properties starting with electronic structure theory. However, the crucial role of temperature and entropy in most materials processes requires a rigorous statistical mechanics approach. In this talk I will describe our recent efforts at bridging the gap between phenomenological theories of materials and first-principles electronic structure predictions. The approach relies on statistical mechanics methods that utilize effective Hamiltonians expressed in terms of mathematically rigorous local descriptors to treat configurational, vibrational and electronic degrees of freedom. Effective Hamiltonians are capable of extrapolating first-principles electronic structure calculations within (kinetic) Monte Carlo simulations, thereby enabling the calculation of equilibrium and non-equilibrium materials properties at finite temperature. I will illustrate how these approaches can be used to predict the dynamic evolution of battery electrodes and high temperature structural materials.