Symposium | A. Advances in Materials Theory for Multiscale Modeling

## [SY-A2]Symposium A-2

Chair: Kenjiro Sugio(Hiroshima Univ., Japan)
Mon. Oct 29, 2018 3:45 PM - 5:30 PM  Room6

# [SY-A2]How to model ordering processes in metallic hydrides? A Tight-Binding Ising modeling proposal and its application to Zr-H

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Modeling metal hydrides is of prime interest in the field of materials for energy, due to these material potential uses as hydrogen storage devices or to their potential formation in nuclear reactors. In particular, zirconium alloys are used in water-cooled nuclear reactor and can be embrittled by hydride precipitation. This motivates developing theoretical tools to model, understand and predict the behavior of zirconium hydrides, and to precise their links to local stresses and mechanical properties. In order to explore the Zr-H phase diagram and to clarify dissolution/precipitation mechanisms and kinetic, one needs thermodynamic simulations such as Monte Carlo approaches. They have to be grounded on an energetic model with a good compromise between precision and numerical cost, and in particular, which is able to characterize order-disorder phenomena on the interstitial H-gap subnetwork of metal hydrides.

To this aim, using the Generalized Perturbation Method based on Tight-Binding Coherent Potential Approximation, we have derived an effective Ising Model, which describes the order energy of the FCC zirconium hydride systems as a sum of interactions of HH pairs. We present here this general approach through the example of Zr-H. The process revealed the predominance of pairwise interaction between third-order hydrogen neighbors. Ability of the pairwise interactions model to characterize hydrogen-vacancy sublattice order has been then established by confrontation to first-principle approaches.