Poster Session | D. Data-Driven and Physics-Informed Materials Discovery and Design

[PO-D2]Poster Session 2

Symposium D

Wed. Oct 31, 2018 5:45 PM - 8:00 PM Poster Hall

[P2-26]Generalized nano-thermodynamic model for predicting size-dependent surface segregation in multi-metal alloy nanoparticles from smaller particles

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Multi-metal alloy nanoparticles (NPs) offer new avenues for exploration and design of nanoscale-properties, e.g., catalytic, electronic and optical, by virtue of their tunable composition. Unfortunately, a method that can aid such exploration by accurately predicting the size-, shape- and composition-dependent elemental distribution associated with nanomaterials is crucially missing. A nano-thermodynamic model based on distribution coefficients Δ is introduced to fill this gap. Δ is employed to predict surface segregation in NPs as a function of the NP size and composition. Interestingly, we find Δ to be independent of size for NPs beyond 2 nm. This key finding motivates the construction of thermodynamic tables for distribution coefficients using segregation observed with one or more NP sizes. The tables can enable accurate prediction of phase diagrams for nanomaterials across a wide-range of sizes. Key concepts of this new theory are demonstrated with Au-Pt-Pd, Ag-Au-Pd and Ni-Pt-Pd, which are found to exhibit complex size-dependent segregation behavior for 2-6 nm NPs and relatively weaker size-dependence beyond 6 nm. Numerically well-converged values of Δ are calculated for small NPs using Monte Carlo simulations in the canonical ensemble. Simulations are based on an embedded atom method (EAM) potential for metal alloys.

[1] S Divi, A Chatterjee, RSC Advances 8, 10409, 2018.