Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Bayesian cluster expansion with lattice parameter dependence for studying surface alloys LE NIU, TIM MUELLER, Johns Hopkins University, Department of Materials Science Engineering — The Bayesian cluster expansion approach has proven to be an efficient method for predicting the structure and properties of materials with substitutional disorder. It is particularly effective for low-symmetry systems such as nanoparticles and surfaces. However for surfaces of solid solutions, the lattice parameter of the surface, and hence the interactions among near-surface atoms, varies with the composition of the underlying bulk material. We demonstrate that surfaces under a variety of strains can be used to train a single cluster expansion that predicts properties as a function of atomic order and surface strain. We have applied this method to study Ni-Pt alloys with up to a monolayer of adsorbed oxygen, an important class of catalysts for the oxygen reduction reaction. Through Monte Carlo simulations, we are able to determine how the structure and properties of these surfaces vary as a function of temperature, composition, chemical potential, and surface strain, enabling both the identification of thermodynamically stable surface structures and the rational design of Pt-Ni surfaces with high catalytic activity.

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Date submitted: 06 Nov 2015 Electronic form version 1.4