Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Alloy surface segregation in reactive environments via density functional theory and atomistic thermodyanamics JOHN KITCHIN, KARSTEN REUTER, MATTHIAS SCHEFFLER, Fritz Haber Institut — The chemical and materials properties of an alloy surface depend sensitively on its detailed surface composition and structure, which in turn can differ substantially from the one of the bulk alloy due to segregation of one species to the surface. Concerning the alloy function e.g. in catalytic or corrosive environments, this surface segregation can furthermore depend on the partial pressures and temperatures in the surrounding if one alloy component interacts more strongly with a gas-phase species than the other. Instead of solely predicting the chemical and materials properties on the basis of the formal bulk composition, this requires a theory that explicitly considers the effect of the reactive environment. As a first step in this endeavor, we are extending the concepts of *ab initio atomistic thermodynamics* to address segregation in binary transition metal alloys in the presence of a reactive gas phase. We apply the approach to the (111) surface of Ag_3Pd in an O_2 atmosphere, and find that contrary to the situation in ultra-high vacuum, Pd segregates to the surface at high oxygen pressures. We discuss the difficulties and possible inaccuracies of the *ab initio atomistic thermodynamic approach* with respect to the limited exploration of configuration space and the steps necessary to proceed beyond it.

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Date submitted: 28 Nov 2004 Electronic form version 1.4