Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Correcting Density Functional Theory for Accurate Predictions of Compound Enthalpies of Formation:Fitted elemental-phase Reference Energies (FERE)[1] VLADAN STEVANOVIC, XIUWEN ZHANG, STEPHAN LANY, National Renewable Energy Laboratory, Golden CO, ALEX ZUNGER, University of Colorado, Boulder CO — The first step in the Inverse Design of materials is the assessment of their thermodynamic stability and the needed growth conditions. The compound enthalpy of formation (ΔH_f) is a quantity that provides these information. However, standard ab-initio approaches are known for their large errors in calculating ΔH_f of semiconducting and insulating compounds. In this talk I will present an approach, based on GGA+U total energies for compounds and fitted elemental-phase reference energies (FERE), that corrects GGA+U for the incomplete error cancellation between compound total energies and those of the pure elements, thereby resulting in ΔH_f values for insulating and semiconducting solids calculated with chemical accuracy. The FERE for 50 chemical elements we fit to a set of 252 measured ΔH_f of binary compounds (pnictides, chalcogenides and halides) and show accurate predictions also when applied to ternary compounds. I will discuss the application of the FERE approach in predicting new compounds, assess the accuracy of such predictions as well as comment on experimental efforts of our collaborators in growing some of the predicted materials.

[1]Funded by DOE through Energy Frontiers Research Centers, Center for Inverse Design

Vladan Stevanovic
National Renewable Energy Laboratory, Golden CO

Date submitted: 11 Nov 2011 Electronic form version 1.4