Correcting Density Functional Theory for Accurate Predictions of Compound Enthalpies of Formation: Fitted elemental-phase Reference Energies (FERE) 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 (\(\Delta H_f\)) is a quantity that provides these information. However, standard ab-initio approaches are known for their large errors in calculating \(\Delta H_f\) 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 \(\Delta H_f\) values for insulating and semiconducting solids calculated with chemical accuracy. The FERE for 50 chemical elements we fit to a set of 252 measured \(\Delta H_f\) 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.

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