

Abstract for an Invited Paper  
for the MAR06 Meeting of  
The American Physical Society

### **Evolutionary approach for determining first-principles model Hamiltonians<sup>1</sup>**

GUS L. W. HART, Northern Arizona University

The ability to perform accurate solid-state calculations based completely on first principles (for relatively small unit cells) has made it possible to develop model Hamiltonians that can be rapidly “searched” for optimal target properties—i.e., true materials-by-design. Recent applications include ferroelectric properties and band-gap engineering. The most difficult step in “training” such model Hamiltonians is making choices for the number and types of parameters in the model that insure the *predictive* power of the model. Based on an evolutionary approach, we have developed an algorithm<sup>2</sup> for selecting the types and number of terms in a Cluster Expansion model for a binary alloy. This approach removes much of the tedium of constructing the model and robustly finds the best possible set of parameters. The approach is general and can be applied to a wide variety of other models as well. I illustrate the success of the new approach first on systems where the best parameter set is known analytically, and second, as applied to several recent “real-world” examples, including (1) the role of long-period-superlattices in the Cu-Pd system, (2) predicting configuration-dependent bulk-moduli in transition-metal carbides and nitrides, (3) predicting optimal superlattice stacking/orientations to engineer desired band-gaps in MgO-ZnO wide gap alloys.

<sup>1</sup>Supported by NSF-0244183; DFG-MU 1648/2 1,2; and a Cottrell College Science Award (Research Corporation).

<sup>2</sup>Gus L. W. Hart, V. Blum, M. J. Walorski, and A. Zunger, *Nature Materials* **4** 391 (2005); V. Blum, Gus L. W. Hart, M. J. Walorski, and A. Zunger, *Phys. Rev. B* **72**, 165111 (2005).