Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Defect engineering of complex semiconductor alloys: $\mathbf{Cu_{2-2x}M_xO_{1-y}X_y}$[1] STEPHAN LANY, National Renewable Energy Laboratory, VLADAN STEVANOVIC, Colorado School of Mines — The electrical properties of semiconductors are generally controlled via doping, i.e., the incorporation of dilute concentrations of aliovalent impurity atoms, whereas the band structure properties (gap, effective masses, optical properties) are manipulated by alloying, i.e., the incorporation of much larger amounts of isovalent elements. Theoretical approaches usually address either doping or alloying, but rarely both problems at the same time. By combining defect supercell calculations, GW quasi-particle energy calculation, and thermodynamic modeling, we study the range of electrical and band structure properties accessible by alloying aliovalent cations (M = Mg, Zn, Cd) and isovalent anions (X = S, Se) in Cu_2O. In order to extend dilute defect models to higher concentrations, we take into account the association/dissociation of defect pairs and complexes, as well as the composition dependence of the band gap and the band edge energies. Considering a composition window for the $Cu_{2-2x}M_xO_{1-y}X_y$ alloys of $0 \leq (x,y) \leq 0.2$, we predict a wide range of possible band gaps from 1.7 to 2.6 eV, and net doping concentrations between $p = 10^{19}$ cm^{-3} and $n = 10^{17}$cm^{-3}, notably achieving type conversion from p- to n-type at Zn or Cd compositions around x = 0.1.

[1]This work is supported as part of the SunShot initiative by the U. S. Department of Energy, Office of Energy Efficiency and Renewable Energy under Contract No. DE-AC36-08GO28308 to NREL.

Stephan Lany
National Renewable Energy Laboratory

Date submitted: 09 Nov 2012 Electronic form version 1.4