Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Asymmetric Cation stoichiometry in Spinels : Site occupancy in Co_2ZnO_4 and Rh_2ZnO_4[1] TULA PAUDEL, S. LANY, A. ZUNGER, A. SIGDEL, A. ZAKUTAYEV, J. PERKINS, D. GINLEY, National Renewable Energy Laboratory, J. BETTINGER, Y. SHI, M. TONEY, SLAC National Accelerator Laboratory, A. NAGARAJA, N. PERRY, T. MASON, North Western University — Cations A and B in A_2BX_4 spinels normally appear in precise 2:1 Daltonian ratio only at low temperature. At finite temperature, they become either A-rich or B-rich, which control dopability of the compound. We survey the experimentally observed stoichiometry asymmetries and describe the first principles framework for calculating these. The results of the calculations compare well with the phase boundary determined from XRD and the site occupancy measured by anomalous-XRD on Co_2ZnO_4 and Rh_2ZnO_4 samples grown in thermodynamic equilibrium. Good comparison between theory and experiment allows us predict the co-existence line in composition range form first principle for other spinels, which in turn can be extended to predict the nature of electrical conductivity of a compound, while designing the material with the desired properties via principle of inverse design.

[1]This work was supported through the Center for Inverse Design, an EFRC funded by the U.S. DOE, Office of Science, Office of BES.

Tula Paudel
National Renewable Energy Laboratory

Date submitted: 13 Dec 2010 Electronic form version 1.4