Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Searching for new transparent conducting oxides(TCO) for energy applications within the A_2BO_4 family using defect calculations for A=Co, Rh, Ir and B=Mg, Ca, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Sr and Cd[1] TULA R. PAUDEL , STEPHAN LANY, ALEX ZUNGER, National Renewable Energy Laboratory — TCO's manifest the unlikely coexistence of optical transparency with electric conductivity and require that electron or hole dopants will not instigate the spontaneous production of defect centres that quench electrons (e.g cation vacancy) or holes (e.g anion vacancy), respectively. We use first principle based methods to screen and design effective hole-TCO's in A_2BO_4 by predicting the concentration of free holes as well as hole-compensating centres as a function of chemical potential and temperature. We search for the "design principles" that control hole production and survival in such materials. This involves calculation of the energy of formation for large number of the defects and dopant as well as the transition levels, which in turn allows us to calculate the career concentration as a function of Fermi energy for a given material. Provided that the data for the group of materials, we would be able to suggest the few best candidates for the p-type TCO in this class of materials.

[1]This work was supported through the Center for Inverse Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences.

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Date submitted: 22 Dec 2009 Electronic form version 1.4