Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Discovering potentially overlooked Filled Tetrahedral Structure compounds by high-throughput first-principles calculation[1] XIUWEN ZHANG, ALEX ZUNGER, National Renewable Energy Lab, SOLID STATE THEORY GROUP TEAM — Filled Tetrahedral Structures (FTS) such as LiZnP are derived from the binary zincblende family by splitting a cation such as Ga in GaP into two lower-valent cations Li+Zn, placing one on the original cation site and the other on one of the empty interstitial sites. Generalizing this process, it is possible to generate a few hundred of ABX compounds. Depending on the position of A, B, and X in the periodic table, the structure of such ABX can deviate from the parent tetrahedral framework. Using high-throughput total-energy calculation in GGA+U we have examined the stable structures and possible metastable structures of a few hundred ABX compounds, establishing the basic regularities relating structure to chemical identity. Their thermodynamical stability has been checked by taking into account the competing binary and ternary phases. We identify dozens of ABX compounds likely to have large band gaps, potentially suitable as solar absorbers and transparent conductors.

[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.

Xiuwen Zhang
National Renewable Energy Lab

Date submitted: 15 Nov 2010 Electronic form version 1.4