Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

**Doping designed half-Heusler insulators** YONGGANG YU, XIUWEN ZHANG, LIPING YU, University of Colorado, Boulder, CO, FENG YAN, A. NAGARAJA, T. O. MASON, Northwestern University, Evanston, IL, ALEX ZUNGER, University of Colorado, Boulder, CO — The 18-valence-electron 1:1:1 compounds of the type III-X-V, IV-X-IV, IV-IX-V and V-IX-IV include thermoelectric materials, topological insulators, and recently a high mobility p-type transparent conductor TaIrGe (arXiv:1406.0872), yet their intrinsic doping trends are poorly known or understood. Using the "modern theory of doping" that addresses via DFT and HSE the thermodynamic formation energies and the DFT-corrected transition levels in the gap, we find the following interesting trends: (1) High atomic number compounds such as TaIrGe made of metallic elements can surprisingly have a large band gap (direct) of $\sim$ 2.5 eV. (2) Half-Heusler such as $A^{(IV)}B^{(X)}C^{(IV)}$ is naturally n-type if its DFT calculated chemical stability field resides within the A-rich or B-rich domain of the stability triangle, while it is p-type if it resides within the C-rich domain. Such calculations provide a good metric. (3) When the B atom [at (1/4,1/4,1/4)] is as large as Ir or Pt, the compound prefers p-type because the C-on-A antisite [such as $Ge_{Ta}^{(1-)}$] is a shallow acceptor producing holes yet the hole-killer donor of B-interstitial is unfavorable. (4) When B=Ni or Co, the compound favors n-type due to the dominance of B-interstitial defects (e.g. TiCoSb). We will show the calculated leading defect types and the dependence of carrier concentrations on chemical conditions for newly predicted half-Heulser insulators. This study is supported by DOE, Office of Science, Basic Energy Science, MSE division grant to CU Boulder.

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Date submitted: 13 Nov 2014 Electronic form version 1.4