Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A. This journal is © The Royal Society of Chemistry 2017

Thermoelectric properties of AMg_2X_2 , AZn_2Sb_2 (A = Ca, Sr, Ba; X = Sb, Bi), and Ba₂ZnX₂ (X = Sb, Bi) Zintl compounds (Supplementary information)

Jifeng Sun and David J. Singh*

Department of Physics and Astronomy, University of Missouri-Columbia, Columbia, MO 65211, USA (Dated: March 30, 2017)

PACS numbers:



FIG. S1: Calculated projected density of states of the eleven compounds using mBJ and SOC.



FIG. S2: Calculated relaxation-time-related electrical conductivity along different directions at 800 K for the $[Mg_2Sb_2]^{2-}$ compounds (a), the $[Mg_2Bi_2]^{2-}$ (b), the $[Zn_2Sb_2]^{2-}$ (c), and the 212 phases (d). Solid lines are *p*-type and dashed lines are *n*-type materials.

* Electronic address: singhdj@missouri.edu