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Thermoelectric properties of AMg_2X_2 , AZn_2Sb_2 ($A = Ca, Sr, Ba$; $X = Sb, Bi$), and Ba_2ZnX_2 ($X = Sb, Bi$) Zintl compounds.¹ JIFENG SUN, DAVID SINGH, Univ of Missouri - Columbia — A theoretical investigation of the electronic structure and transport properties of eleven Zintl compounds including nine 122 phases (AMg_2X_2 , AZn_2Sb_2 ($A = Ca, Sr, Ba$; $X = Sb, Bi$)) and two 212 phases (Ba_2ZnX_2 ($X = Sb, Bi$)) are reported. The electronic structures and electrical transport properties are studied using *ab initio* calculations and semi-classical Boltzmann theory within the constant relaxation time approximation. Band structure calculations using mBJ potential with spin-orbit coupling verify the semiconducting behavior for all of the compounds. The Seebeck coefficient, electrical conductivity and power factor results predict that the n-type 122 phase having better thermoelectric performance than p-type material due to the larger multivalley degeneracy at and near conduction band minimum compared with valence band maximum. The general performance of 212 phase is inferior to the 122 phase, with Ba_2ZnSb_2 compound showing better performance. The anisotropy character of Seebeck coefficients and electrical conductivity is also discussed.

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