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### **Thermoelectric Properties of Complex Zintl Phases**

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Complex Zintl phases make ideal thermoelectric materials because they can exhibit the necessary “electron-crystal, phonon-glass” properties required for high thermoelectric efficiency. Complex crystal structures can lead to high thermoelectric figure of merit ( $zT$ ) by having extraordinarily low lattice thermal conductivity. A recent example is the discovery that  $\text{Yb}_{14}\text{MnSb}_{11}$ , a complex Zintl compound, has twice the  $zT$  as the SiGe based material currently in use at NASA. The high temperature (300K - 1300K) electronic properties of  $\text{Yb}_{14}\text{MnSb}_{11}$  can be understood using models for heavily doped semiconductors. The free hole concentration, confirmed by Hall effect measurements, is set by the electron counting rules of Zintl and the valence of the transition metal ( $\text{Mn}^{+2}$ ). Substitution of nonmagnetic  $\text{Zn}^{+2}$  for the magnetic  $\text{Mn}^{+2}$  reduces the spin-disorder scattering and leads to increased  $zT$  (10%). The reduction of spin-disorder scattering is consistent with the picture of  $\text{Yb}_{14}\text{MnSb}_{11}$  as an underscreened Kondo lattice as derived from low temperature measurements. The hole concentration can be reduced by the substitution of  $\text{Al}^{+3}$  for  $\text{Mn}^{+2}$ , which leads to an increase in the Seebeck coefficient and electrical resistivity consistent with models for degenerate semiconductors. This leads to further improvements (about 25%) in  $zT$  and a reduction in the temperature where the  $zT$  peaks. The peak in  $zT$  is due to the onset of minority carrier conduction and can be correlated with reduction in Seebeck coefficient, increase in electrical conductivity and increase in thermal conductivity due to bipolar thermal conduction.