Talk

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Zintl Phases as Thermoelectric Semiconductors G. Jeffrey Snyder Northwestern Universitywww.thermoelectrics.matsci.northwestern.edu We often understand the physical properties of Zintl Phases by considering the perfect crystalline material that is defect free. Yet this perfect, stoichiometric (valence balanced) crystal is an intrinsic semiconductor with equal number of electrons and holes. To make a n-type or p-type semiconductor we typically use point defects to introduce a slight valence imbalance that leads to excess electrons or holes. Often intrinsic defects such as vacancies, interstials or antisite defects, provide the necessary carriers to make the material a good thermoelectric (e.g. Zn4Sb3, Bi2Te3-Sb2Te3, YbxCoSb3, etc.). Most materials, however, require extrinsic dopants to be a good thermoelectric and intrinsic defects only make it more complicated. Sometimes intrinsic defects are so prevalent they are killer defects that prevent any dopant from making the material n-type or p-type.Point defects can also make gradual but profound changes to the band structure compared to the defect free compound. This includes increasing band gap for higher temperature application, reducing conductivity mass for higher mobility or band convergence for dramatic increase in density of states (Pb(Se,Te), Mg2(Si,Sn), Bi2Te3-Sb2Te3,). In principle all of these defects can be better controlled by engineering chemical potentials through phase boundaries. Even the Ni content MNiSn (M = Ti, Zr, Hf) Half-Heusler thermoelectrics can be sufficiently altered to make substantial differences in electronic properties. The excess Ni produces impurity states in the band gap that changes the effective band gap and leads to additional electron and phonon scattering. References[1] Zeier, Snyder, et al. Angew. Chem. Int. Ed. 55, 6826 (2016)

Monday, June 13, 2022 11:00am - 12:00pm

Big Seminar Room B - Sunstone Building

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