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The Use of Zintl Chemistry for Understanding Thermoelectric Half Heusler Materials

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ABSTRACT:

The thermal and electrical properties of complex semiconductors may be complicated with many contributing mechanisms, but with the aid of solid-state chemistry principles [1] several trends and unusual properties can be understood. N-type XNiSn (X = Ti, Zr, Hf) half-Heusler (HH) compounds, which can be described as semiconductors using a Zintl formalism [2], possess excellent thermoelectric properties. In contrast, p type XNiSn HH compounds have poor figures of merit, zT, compared to XCoSb compounds. The high zT values in n-type XNiSn (X = Ti, Zr, Hf) HH compounds can be traced to an effective suppression of the bipolar effect [3] in the thermoelectric transport properties due to the presence of interstitial Ni states that make up the valence band. These principles can also help understand defects. The evidence for interstitial Ni in XNiSn Half-Heusler thermoelectrics could also be used to understand and control doping, thermal and electrical transport and even microstructure such as the full-Heusler inclusions found experimentally. Using these and examples from Zintl-compounds AZn2Sb2 [4] and Ca5M2Sb6 I will describe how we attempt to use Zintl Chemistry to understand, explain and ultimately predict the effects of defects.

BIOGRAPHY:

G. Jeffrey Snyder is a Professor of Materials Science and Engineering at Northwestern University in Evanston Illinois. His interests are focused on the materials physics and chemistry for thermoelectric engineering, such as band engineering, design of complex Zintl compounds and use of nanostructured composites. His interdisciplinary approach to thermoelectrics stems from studies of Solid State Chemistry at Cornell University and the Max Planck Institute for solid state research, Applied Physics at Stanford University and thermoelectric materials & device engineering at NASA/Jet Propulsion Laboratory (JPL) and California Institute of Technology (Caltech). He started working in thermoelectrics in 1997 after joining the Thermoelectrics group at JPL. In 2006 he started the Caltech thermoelectrics group. In 2002 he served as technical program chair for the ICT in Long Beach California. He has served on the board of ITS since 2007 and as treasurer since 2010. He has over 300 publications in thermoelectrics and mentored several students and postdocs in the field including three Goldsmid and two ITS Young Investigator Award winners.