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SEMINAR

Why interstitial Ni makes Half-Heusler ZrNiSn a good n-type but poor p-type Thermoelectric

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Moderator	Corsin Battaglia
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Abstract

N-type *X*NiSn (*X* = Ti, Zr, Hf) Half-Heusler (HH) compounds, which can be described as semiconductors using a Zintl formalism, possess excellent thermoelectric properties. In contrast, *p*-type *X*NiSn HH compounds have poor figures of merit, *zT,* compared to *X*CoSb compounds. The high *zT* values in *n*-type *X*NiSn (*X* = Ti, Zr, Hf) HH compounds can be traced to an effective suppression of the bipolar effect in the thermoelectric transport properties due to the presence of interstitial Ni states that make up the valence band. Normally the *zT* is limited by the suppression of the thermopower at high temperatures by thermal excitation of carriers of opposite sign (bipolar effect). This can be roughly described by the Goldsmid-Sharp equation: $E_g = 2eS_{max}T_{max}$ relating the band gap and the temperature where the thermopower peaks.[1] The study of n- and *p*-type HH *X*NiSn solid solutions show that the large mobility difference between electrons and holes in *X*NiSn results in a significant correction to the Goldsmid-Sharp formula. This finding explains the difference in the thermopower band gap between *n*-type and *p*-type HH enabling high *zT* values in *n*-type *X*NiSn (*X* = Ti, Zr, Hf) HH compounds. Thus the low mobility valence band acts as a trap for minority carriers *n*-type *X*NiSn.

[1] Gibbs, Schmitt, Kim, Felser, Snyder et. al. *Materials Horizons* **2**, 68 (2015); *Applied Physics Letters* **106**, 022112 (2015)

Bio

G. Jeffrey Snyder obtained his B.S. degree in physics, chemistry and mathematics at Cornell University (1991) focusing on solid state chemistry which he continued during a two year stay at the Max Planck Institut FKF (Festkörperforschung) in Stuttgart, Germany. He received his Ph.D. in applied physics from Stanford University (1997) where he studied magnetic and magneto-electrical transport properties of

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metallic perovskites as a Hertz Fellow. He was a Senior Member of the Technical Staff in the thermoelectrics group at NASA's Jet Propulsion Laboratory for 9 years (1997-2006) and as a Faculty Associate in materials science at the California Institute of Technology (Caltech) 2006-2014 where he focused on thermoelectric materials and devices. His interests include the discovery of new Zintl phase thermoelectric materials and nanostructured thermoelectric composites using bulk processing, band structure engineering and thermoelectric performance optimization. Dr. Snyder has published over 200 articles, book chapters and patents. He served as treasurer of the international thermoelectric society and vice president of the international thermoelectric academy.

Dr. Snyder is one of the world's most prominent scientists in the rapidly growing field of thermoelectrics. His 2008 review article in *Nature Materials*, is used internationally to instruct many new students, and introduce the essentials of thermoelectricity to a multi-disciplinary audience. It is the most cited article in thermoelectrics in 2013.