

Abstract Submitted  
for the MAR14 Meeting of  
The American Physical Society

**Electronic structure of Zr-Ni-Sn systems: the role of nanostructures and clustering in Half-Heusler and Heusler limits**<sup>1</sup> DAT DO, S.D. MAHANTI, Michigan State University — Half-Heusler and Heusler compounds have been of great interest for several decades for thermoelectric, magnetic, half-metallic and many other interesting properties. Among these systems, Zr-Ni-Sn compounds are interesting thermoelectrics which can go from semiconducting half-Heusler (HH) limit, ZrNiSn, to metallic Heusler limit (FH), ZrNi<sub>2</sub>Sn. Recently Makogo et al. [J. Am. Chem. Soc. 133, 18843 (2011)] found that dramatic improvement in the thermoelectric power factor of HH can be achieved by putting excess Ni into the system. This was attributed to an energy filtering mechanism due to the formation of FH nanostructures in the HH matrix. Using density functional theory we have investigated clustering and nanostructure formation in HH<sub>1-x</sub>FH<sub>x</sub> systems near the HH and FH ends. These results and the effects of nanostructures on electronic structure and thermoelectric properties will be discussed in this talk.

<sup>1</sup>This work was supported by the Center for Revolutionary Materials for Solid State Energy Conversion, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences

Dat Do  
Michigan State University

Date submitted: 15 Nov 2013

Electronic form version 1.4