Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Reducing the lattice thermal conductivity of the rocksalt I-V-VI_2 compounds[1] MICHELE NIELSEN, SUNPHIL KIM, Department of Mechanical and Aerospace Engineering, Ohio State University, Columbus, Ohio 43210, MATTHIAS WUTTIG, FELIX LANGE, I. Physikalisches Institut (IA), RWTH Aachen University, 52056 Aachen, Germany, JOSEPH HEREMANS, Department of Mechanical and Aerospace Engineering, Department of Physics, Ohio State University, Columbus, Ohio 43210 — Reducing the lattice thermal conductivity is a crucial task in the optimization of the thermoelectric figure of merit. Recent theoretical calculations [1] have revealed the presence marginally stable acoustic phonons which have extremely large Grünesien parameters which result in a strong anharmonicity in heat-carrying acoustic phonon branches of select rocksalt I-V-VI2 compounds as a result of lone pair electrons on group V elements. Here, we present a new simple method of mapping Grünesien parameters, using readily available information on the ionization and the hybridization of the chemical bonds involved, and avoiding extensive numerical simulations. Additionally, we present current advances in doping on alkali based compounds which have inexpensive and non-toxic starting constituents.

[1] Michele D. Nielsen, Vidvuds Ozolins and Joseph P. Heremans, Lone pair electrons minimize lattice thermal conductivity, Energy Environ. Sci., 6, 570 – 578 (2013)

[1]This work is supported as part of the "Revolutionary Materials for Solid State Energy Conversion (RMSSEC)," an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science.

Michele Nielsen
Ohio State University

Date submitted: 14 Nov 2013 Electronic form version 1.4