Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Acoustic-optical phonon branch crossings and lattice thermal transport in $La_3Cu_3X_4$ (X = P, As, Sb, and Bi) systems[1] TRIBHUWAN PANDEY, CARLOS A. POLANCO, LUCAS LINDSAY, DAVID S. PARKER, Oak Ridge National Laboratory — Thermoelectric properties of $La_3Cu_3X_4$ (X = P, As, Sb, and Bi) compounds are examined using first-principles density functional theory and Boltzmann transport calculations. It is well known that the lattice thermal conductivity (κ_l) of bulk materials typically decreases with increasing atomic masses of the constituent elements. In this study, however, we observe contrary behavior: lighter mass, larger sound velocity $La_3Cu_3P_4$ and $La_3Cu_3As_4$ systems have lower κ_l than heavier mass, smaller sound velocity $La_3Cu_3Sb_4$ and $La_3Cu_3Bi_4$ systems. Analysis of three phonon scattering rates and other phonon properties demonstrate that the trend in κ_l behavior is governed by Grüneisen parameters, a measure of phonon anharmonicity. The Grüneisen parameters and lower κ_l of the P and As compounds are closely related to an avoided crossing between the lowest optical branches and the longitudinal acoustic branch, which results in abrupt changes in Grüneisen parameters. Additionally, electronic structure calculations show heavy and light bands near the band edges, which lead to large power factors important for good thermoelectric performance.

[1]T. P, C. A. P, L. L. and D. S. P. acknowledge support from the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division.

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Date submitted: 09 Nov 2016 Electronic form version 1.4