Acoustic-optical phonon branch crossings and lattice thermal transport in La$_3$Cu$_3$X$_4$ (X = P, As, Sb, and Bi) systems$^1$ TRIBHUVAN PANDEY, CARLOS A. POLANCO, LUCAS LINDSAY, DAVID S. PARKER, Oak Ridge National Laboratory — Thermoelectric properties of La$_3$Cu$_3$X$_4$ (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 ($\kappa_l$) 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$_3$Cu$_3$P$_4$ and La$_3$Cu$_3$As$_4$ systems have lower $\kappa_l$ than heavier mass, smaller sound velocity La$_3$Cu$_3$Sb$_4$ and La$_3$Cu$_3$Bi$_4$ systems. Analysis of three phonon scattering rates and other phonon properties demonstrate that the trend in $\kappa_l$ behavior is governed by Grüneisen parameters, a measure of phonon anharmonicity. The Grüneisen parameters and lower $\kappa_l$ 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.


Tribhuwan Pandey
Oak Ridge National Lab

Date submitted: 09 Nov 2016