Abstract Submitted
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Anomalous pressure dependence of thermal conductivities of large mass ratio compounds L. LINDSAY, Oak Ridge National Laboratory, D.A. BROIDO, Boston College, J. CARRETE, N. MINGO, CEA-Grenoble, T.L. REINECKE, U.S. Naval Research Laboratory — The lattice thermal conductivities (k) of binary compound materials are examined as a function of hydrostatic pressure, P, using a first-principles approach. Compound materials with relatively small mass ratios, such as MgO, show an increase in k with P, consistent with measurements. Conversely, compounds with large mass ratios (*e.g.*, BSb, BAs, BeTe, BeSe) exhibit decreasing k with increasing P, a behavior that cannot be understood using simple theories of k. This anomalous P dependence of k arises from the fundamentally different nature of the intrinsic scattering processes for heat-carrying acoustic phonons in large mass ratio compounds compared to those with small mass ratios. This work demonstrates the power of first principles methods for thermal properties and advances the understanding of thermal transport in non-metals. * * * L. L. acknowledges support from the U. S. Department of Energy, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division for work done at ORNL. D.A.B acknowledges support from the National Science Foundation under Grant No. 1402949. NM and JC acknowledge support from Institut Carnot through project SIEVE. T.L.R. acknowledges support from ONR and DARPA.

Lucas Lindsay
Oak Ridge National Laboratory

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