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**First principles study of lattice thermal conductivity and large isotope effect in materials**[1] DAVID BROIDO, Boston College, LUCAS LINDSAY, NRC Research Associate, Naval Research Laboratory, TOM REINECKE, Naval Research Laboratory — The isotope effect—the percent enhancement to a material's lattice thermal conductivity, $k$, with isotopic purification—depends on the interplay between phonon-isotope and phonon-phonon scattering. Diamond is known to have the largest measured room temperature (RT) isotope effect of any bulk crystal, achieving a $k$ enhancement of 50%. Using an *ab initio* Boltzmann transport equation approach, we have identified several other materials with far larger RT isotope effects [1]. In particular, we find that germanium carbide (GeC) and beryllium selenide (BeSe) have RT isotope effects of 450%, almost an order of magnitude higher than that in diamond. Isotopic purification in these materials gives surprisingly high intrinsic RT $k$ values, over 1500 $\mathrm{Wm^{-1}K^{-1}}$ for GeC and over 600 $\mathrm{Wm^{-1}\ K^{-1}}$ for BeSe, well above those of the best metals. These large values stem from fundamental material properties that give both enhanced phonon scattering by isotopes and weak anharmonic phonon-phonon scattering. The physical insights discussed in this work provide guidance for efficient manipulation of thermal transport properties of compound semiconductors through isotopic modification.

[1] L. Lindsay, D. A. Broido and T. L. Reinecke, Phys. Rev. B 88, 144306 (2013).

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