Abstract Submitted
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First principles determination of ultra-high thermal conductivity fo Boron Arsenide: A competitor for diamond?[1] LUCAS LINDSAY, NRC Research Associate at the U.S. Naval Research Laboratory, DAVID BROIDO, Department of Physics, Boston College, TOM REINECKE, U.S. Naval Research Laboratory, LINDSAY COLLABORATION — We have calculated the thermal conductivities (k) of cubic III-V boron compounds using a predictive first principles approach. Boron Arsenide (BAs) is found to have a remarkable room temperature k over 2000$\mathrm{Wm^{-1}K^{-1}}$; this is comparable to those in diamond and graphite, which are the highest bulk values known. We trace this behavior in BAs to an interplay of certain basic vibrational properties that lie outside of the conventional guidelines in searching for high k materials. We also find that cubic BN and BSb will have high k with isotopic purification. This work provides new insight into the nature of thermal transport at a quantitative level and predicts a new ultra-high k material of potential interest for passive cooling applications.

[1] L. Lindsay, D. A. Broido, and T. L. Reinecke, Phys. Rev. Lett. 111, 025901 (2013).

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Lucas Lindsay
NRC Research Associate at the U.S. Naval Research Laboratory

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