Abstract Submitted
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Enhanced thermal conductivity and isotope effect in single-layer hexagonal boron nitride[1] DAVID BROIDO, Boston College, LUCAS LINDSAY, Naval Research Laboratory — We have calculated the lattice thermal conductivity, k, of both naturally occurring and isotopically enriched single layers of hexagonal boron nitride (h-BN) as well as bulk h-BN using an exact numerical solution of the Boltzmann transport equation for phonons [1]. Good agreement is obtained with measured bulk h-BN data [2], and the stronger phonon-phonon scattering identified in these systems explains why their k values are significantly lower than those in graphene and graphite. A reduction in such scattering in the single layer arising mainly from a symmetry-based selection rule leads to a substantial increase in$k$, with calculated room temperature values of more than 600 W/m-K. Additional enhancement is obtained from isotopic enrichment, which exhibits a strong peak as a function of temperature, with magnitude growing rapidly with crystallite size. [1] L. Lindsay and D. A. Broido, Phys. Rev. B 84, 155421 (2011). [2] E. K. Sichel, R. E. Miller, M. S. Abrahams, and C. J. Buiocchi, Phys. Rev. B 13, 4607 (1976).

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