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Ab initio theory of thermal properties of germanane MATTHEW HEINE, Boston College, LUCAS LINDSAY, Oak Ridge National Lab, JESÚS CARRETE, NATALIO MINGO, LITEN, CEA-Grenoble, OLLE HELLMAN, Linköping University, DAVID BROIDO, Boston College — Germanane(GeH) is a germanium based hydrogen-terminated multi-layered graphane analogue semiconductor, which may be a promising thermoelectric due to its high electron mobility and the capability to tune its transport properties [1]. We have performed first principles calculations of the thermal properties of germanane. Harmonic and anharmonic interatomic force constants are calculated within the framework of density functional theory, from which phonon dispersions, specific heat, thermal expansion are obtained. The phonon Boltzmann equation is solved to obtain the lattice thermal conductivity. The disparity in constituent masses in GeH gives phonon modes that are distinctly Ge or H in character and causes the specific heat not to saturate until much higher temperatures than in bulk Ge. Weak interlayer bonding and strong phonon-phonon scattering result in highly anisotropic and quite low intrinsic lattice thermal conductivity compared to Ge.
[1] E. Bianco et. al., ACS Nano 7, 4414-4421 (2013).

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