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Studying phonon lifetimes and heat conductivity of wurtzite aluminum nitride

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Phonon lifetimes and heat conductivity of wurtzite aluminum nitride has been studied by two different computational methodologies. The first method uses a molecular dynamics equilibrium Green-Kubo formalism to compute the thermal conductivity. It requires large simulation cells and long simulation times, practically accessible using classical forcefield methods. The method can be extended to calculate wavevector and frequency resolved thermal conductivities and phonon lifetimes by projecting the heat flux onto the vibrational modes. The second approach used in the present study is to calculate these anharmonic processes by explicitly evaluating the anharmonic force constants. This is done using the PhononA package (Parlinski, Ab initio determination of anharmonic phonon peaks, 2018) and is based on forces extracted from supercell calculations.

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