# Supplementary Information for Phonon Thermal Transport in Irida-Graphene via Non-equilibrium Molecular Dynamics Simulations

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## I. LATTICE THERMAL CONDUCTIVITY OF GRAPHENE WITH REBO POTENTIAL

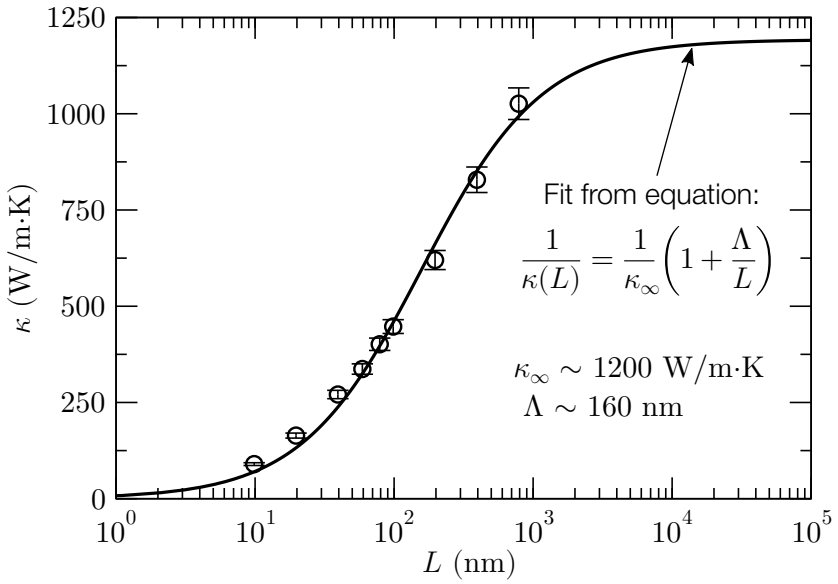


FIG. S1. Thermal conductivity of graphene as a function of sample length using the second-generation REBO potential. Data points are from RNEMD simulations, and lines are from Eq. (4) of the main text.

Figure S1 shows the thermal conductivity as a function of the graphene system length obtained using the second-generation REBO potential [1]. This value falls within the range of other molecular dynamics simulation results that used the same potential to calculate the thermal conductivity of graphene [2, 3], but it is lower than experimental results ($\sim 1500 - 5800$ W/mK) [4–8]. This is likely

due to the fact that the REBO potential does not reproduce the optical phonons correctly [9, 10], which would change the phase space for phonon-phonon scattering and thus change the phonon relaxation time [11, 12].

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