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Effects of vdW and Electrostatic Interactions on Phonon Velocity and Thermal Transport in Polymers VAHID RASHIDI, ELEANOR COYLE, JOHN KIEFFER, KEVIN PIPE, University of Michigan — Bulk amorphous polymers typically have a low thermal conductivity (˜0.2 W/mK). This low thermal conductivity is believed to be due to weak inter-chain interactions, e.g., van der Waals and electrostatic. Heat transfer along polymer chains, however, is considered very robust due to strong covalent bonds between the atoms. In this work we show that this explanation does not give a clear picture of precisely what contributes to heat transfer in various polymers with different structures. Here we show that the abundance of vdW and electrostatic interactions can greatly impact heat transfer in polymers at room temperature. Through molecular dynamics calculations, we show that the propagation velocities of acoustic phonons at moderate frequencies (˜1THz), which contribute significantly to heat transfer at room temperature, are much higher when non-bonding interactions are present in the system versus when they are excluded. This relationship has important implications for designing amorphous polymers with high thermal conductivity.

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