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Engineering thermal conductivity in polymer blends[1] VAHID RASHIDI, ELEANOR COYLE, JOHN KIEFFER, KEVIN PIPE, Univ of Michigan - Ann Arbor — Weak inter-chain bonding in polymers is believed to be a bottleneck for both thermal conductivity and mechanical strength. Most polymers have low thermal conductivity (˜0.1 W/mK), hindering their performance in applications for which thermal management is critical (e.g., electronics packaging). In this work, we use computational methods to study how hydrogen bonding between polymer chains as well as water content can be used to engineer thermal transport in bulk polymers. We examine how changes in the number of hydrogen bonds, chain elongation, density, and vibrational density of states correlate with changes in thermal conductivity for polymer blends composed of different relative constituent fractions. We also consider the effects of bond strength, tacticity, and polymer chain mass. For certain blend fractions, we observe large increases in thermal conductivity, and we analyze these increases in terms of modifications to chain chemistry (e.g., inter-chain bonding) and chain morphology (e.g., chain alignment and radius of gyration). We observe that increasing the number of hydrogen bonds in the system results in better packing as well as better chain alignment and elongation that contribute to enhanced thermal conductivity.

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