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Thermal Transport in C60 Molecular Crystals Above Room Temperature[1] CAROLINE S. GORHAM, ALAN J. H. MCGAUGHEY, Department of Mechanical Engineering, Carnegie Mellon University — The thermal conductivity of solid fullerene molecular systems has garnered significant interest as an example of materials whose thermal transport is dominated by Einstein-type oscillators. Using classical molecular dynamics simulations, this study isolates the roles of intramolecular and intermolecular vibrational degrees of freedom on the bulk thermal conductivity of the face-centered cubic C_{60} molecular crystal. The Green-Kubo method is used to predict the bulk thermal conductivity. The contributions to thermal transport resulting from collective motions of the molecules, molecular rotations, and intramolecular vibrations are isolated using non-equilibrium methods. These contributions are interpreted using a Debye model, a nearest-neighbor resistance network, and Allen-Feldman theory.

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