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Between Crystal and Glass: Thermal Transport in C60 Molecular Crystals[1] SIMON LU, SUSHANT KUMAR, ALAN MCGAUGHEY, Department of Mechanical Engineering, Carnegie Mellon University — Molecular crystals of the fullerene C60 and its derivatives [e.g., phenyl-C61-butyric acid methyl ester (PCBM)] are candidate materials for use in photovoltaics and thermoelectrics. In thermoelectrics, their usefulness is due in part to their exceptionally low thermal conductivities (0.4 W/m-K for C60 and 0.05 W/m-K for PCBM) at room temperature. Little is known regarding the microscopic physics underlying these low thermal conductivities. An important question is whether thermal transport in the C60 molecular crystal is (i) crystal-like, where energy is transported as collective vibrations of the centers of mass of the molecules, or (ii) amorphous-like, where energy diffuses from molecule to molecule. We use molecular dynamics (MD) simulations and the Green-Kubo method to probe this question by predicting the relative contributions of crystal-like and amorphous-like transport to the thermal conductivity of the C60 molecular crystal. To isolate crystal-like transport, we perform simulations on C60 crystals where molecular rotations and intra-molecular vibrations are prohibited. To isolate amorphous-like transport, we fix the centers of mass of the molecules. We compare the MD results to predictions from a fully diffusive network resistance model.

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