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Modeling Thermal Conductivity of Organic-Inorganic Hybrid Perovskite Methylamine Lead Iodide GAGE T. MAREK, Dept. of Physics, John Carroll University, ANTON KOVALSKY, LILI WANG, CLEMENS BURDA, Dept. of Chemistry, Case Western Reserve University, JEFFREY S. DYCK, Dept. of Physics, John Carroll University — Organic-Inorganic hybrid Perovskite Methylamine Lead Iodide ($CH_3NH_3PbI_3$) is being studied for its promise as high quality photovoltaic material. This material provides advantages like the use of inexpensive base materials, similar manufacturing to modern thin-film materials, and has shown relatively high conversion efficiency of 16%. For use in real world application the effect of radiant heat from the sun cannot be ignored as it has profound effects on output efficiency due to thermally-induced structural degradation, and photovoltage reduction. Thermal conductivity measurements on dense, pressed pellets of polycrystalline $CH_3NH_3PbI_3$ were taken over the temperature range 10-300K, and extremely low thermal conductivity values were found. It is a compelling question whether or not the local vibrational modes of the methylamine ion are responsible for the low thermal conductivity. The data were compared to a simple model of the lattice thermal conductivity that takes into account various mechanisms of phonon scattering. We find that we obtain excellent fits of the data to the model by taking into account only point defect, grain boundary, and three-phonon Umklapp scattering. In particular, we do not find that it is necessary to include resonant phonon scattering due to the methylamine ion.

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