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Phonon properties and slow organic-to-inorganic sub-lattice thermalization in hybrid perovskites MARIA CHAN, Argonne National Lab, ANGELA CHANG, Northwestern University, YI XIA, SRIDHAR SADASIVAM, PEIJUN GUO, ALPER KINACI, Argonne National Lab, HAO-WU LIN, National Tsing-Hua University, PIERRE DARANCET, RICHARD SCHALLER, Argonne National Lab — Organic-inorganic hybrid perovskite halide compounds have been investigated extensively for photovoltaics (PVs) and related applications. The thermal transport properties of hybrid perovskites, including phonon-carrier and phonon-phonon interactions, are of significance for their PV and solar thermoelectric applications. The interlocking organic and inorganic sublattices can be thought of as an extreme form of nanostructuring. A result of this nanostructuring is the large gap in phonon frequencies between the organic and inorganic sublattices, which is expected to create bottlenecks in phonon equilibration. In this work, we use a combination of ultrafast spectroscopy including photoluminescence and transient absorption, as well as first principles density functional theory (DFT), ab initio molecular dynamics calculations, phonon lifetimes derived from DFT force constants, and non-equilibrium phonon dynamics accounting for phonon lifetimes, to determine the phonon and charge interaction processes. We find evidence that thermalization of carriers occur at an atypically slow 50-100 ps time scale owing to the complex interplay between electronic and phonon excitations (A. Y. Chang et al, Advanced Energy Materials 2016, DOI: 10.1002/aenm.201600422).

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