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The dynamics and structure of methylammonium ions in hybrid halide perovskites; a combined neutron scattering and first-principles study LINDA HUNG, National Institute of Standards and Technology, BAHAR IPEK, CRAIG BROWN, National Institute of Standards and Technology and University of Delaware, TANER YILDIRIM, National Institute of Standards and Technology, BENJAMIN FOLEY, TIANRAN CHEN, JOSHUA CHOI, SEUNGHUN LEE, University of Virginia — We study the influence of the methylammonium cations on the structure and dynamics of $CH_3NH_3PbI_3$ through a combined first-principles computation and neutron scattering approach. Temperature-dependent powder diffraction indicates phase transitions near 160 K and 300 K, and the lattice parameters, bond angles, and atomic positions are determined. Density-functional theory (DFT) calculations confirm that the most stable form of the orthorhombic phase is non-polar, although the energy difference compared to ferroelectric orientations is only a few meV per atom. Inelastic neutron scattering (INS) spectra are compared to first-principles computations, and significant multi-phonon scattering is observed. Computations predict that lattice dynamics are sensitive to the orientation of the dipoles, and suggest that vibrational spectroscopy may be used as a probe of the local dipole ordering. In particular, the twisting mode along the C-N bond is a single sharp peak near 39 meV for the non-polar orientation and in our INS measurements, but splits into separate peaks for certain ferroelectric orientations.

Linda Hung
National Institute of Standards and Technology

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