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Local polar fluctuations in lead halide perovskite crystals YINSHENG GUO, Columbia University, OMER YAFFE, Weizmann Institute of Science, LIANG TAN, University of Pennsylvania, DAVID EGGER, Weizmann Institute of Science, TREVOR HULL, Columbia University, CONSTANTINOS STOUMPOS, Northwestern University, FAN ZHENG, University of Pennsylvania, TONY HEINZ, Stanford University, LEEOR KRONIK, Weizmann Institute of Science, MERCOURI KANATZIDIS, Northwestern University, JONATHAN OWEN, Columbia University, ANDREW RAPPE, University of Pennsylvania, MARCOS PIMENTA, Universidade Federal de Minas Gerais, LOUIS BRUS, Columbia University — Hybrid lead-halide perovskites have emerged as an excellent class of photovoltaic materials. Recent reports suggest that the organic molecular cation is responsible for local polar fluctuations that inhibit carrier recombination. We combine low frequency Raman scattering with first-principles molecular dynamics (MD) to study the fundamental nature of these local polar fluctuations. Our observations of a strong central peak in both hybrid ($CH_3NH_3PbBr_3$) and all-inorganic ($CsPbBr_3$) lead-halide perovskites show that anharmonic, local polar fluctuations are intrinsic to the general lead-halide perovskite structure, and not unique to the dipolar organic cation. MD simulations show that head-to-head Cs motion coupled to Br face expansion, on a few hundred femtosecond time scale, drives the local polar fluctuations in $CsPbBr_3$.

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