

Abstract Submitted
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Impact of Large Thermal Motion on Critical Properties of Perovskite Photovoltaic Systems T. A. TYSON, New Jersey Institute of Technology, W. GAO, University of South Florida, Y.-S. CHEN, University of Chicago, S. GHOSE, Brookhaven National Laboratory, Y. YAN, New Jersey Institute of Technology — To gain a fundamental understanding of their properties on an atomic level, we investigate single crystals of $\text{CH}_3\text{NH}_3\text{PbI}_3$ with a narrow transition (~ 5 K) near 327 K. We show that the ADPs for I ions yield extended flat regions in the potential wells consistent with the measured large thermal expansion parameter. We also show that the intrinsically enhanced freedom of motion of the iodine atoms enables large deformations. This flexibility (softness) of the atomic structure results in highly localized atomic relaxation about defects and hence accounts for both the high carrier mobility as well as the structural instability.

T. A. Tyson
New Jersey Institute of Technology

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