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Entropy-driven structural transition and kinetic trapping in formamidinium lead iodide perovskite TIANRAN CHEN, Department of Physics, University of Virginia, BENJAMIN FOLEY, Department of Chemical Engineering, University of Virginia, CHANGWON PARK, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, CRAIG BROWN, LELAND HARRIGER, NIST Center for Neutron Research, National Institute of Standards and Technology, JOOSEOP LEE, JACOB RUFF, Cornell High Energy Synchrotron Source, Cornell University, MINA YOON, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, JOSHUA CHOI, Department of Chemical Engineering, University of Virginia, SEUNG-HUN LEE, Department of Physics, University of Virginia — A challenge of hybrid perovskite solar cells is device instability, which calls for an understanding of the perovskite structural stability and phase transitions. Using neutron diffraction and first-principles calculations on formamidinium lead iodide ($FAPbI_3$), we show that the entropy contribution to the Gibbs free energy caused by isotropic rotations of the FA^+ cation plays a crucial role in the cubic-to-hexagonal structural phase transition. Furthermore, we observe that the cubic-to-hexagonal phase transition exhibits a large thermal hysteresis. Our first-principles calculations confirm the existence of a potential barrier between the cubic and hexagonal structures, which provides an explanation for the observed thermal hysteresis. By exploiting the potential barrier, we demonstrate kinetic trapping of the photovoltaic pseudo-cubic phase at low temperatures by thermal quenching [1].
[1] Chen *et al. Sci. Adv.* 2016;2: e1601650 21 October 2016

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