

Abstract Submitted
for the 4CF17 Meeting of
The American Physical Society

Glassy Behavior in a Crystalline Lattice: Substituted Hybrid Perovskites¹ EVE MOZUR, Colorado State Univ, ANNALISE MAUGHAN, Colorado State University, YONGQIANG CHENG, ASHFIA HUQ, NIINA JALARVO, LUKE DAEMEN, Oak Ridge National Laboratory, JAMES NEILSON, Colorado State University — Hybrid perovskites are at the forefront of research for the next generation of semiconductors for solar cells, even though the fundamental physics behind their electronic properties are not well understood. The presence of a dynamic organic cation is typically thought to localize charge carriers, but hybrid perovskites preform competitively with conventional semiconductors. Therefore, many questions remain about the influence of an organic cation on the dynamics, structure, and phase behavior of a crystalline framework. We have characterized the crystallographic and dynamic behavior of the series $(\text{CH}_3\text{NH}_3)_{1-x}\text{Cs}_x\text{PbBr}_3$. Cs^+ substitution leads to the formation of an orientational glass, which can be described as a disordered molecular sublattice coupled to a periodic inorganic framework. We attribute the glassiness of the lattice to geometric strain at the substituted site. In $(\text{CH}_3\text{NH}_3)_{0.8}\text{Cs}_{0.2}\text{PbBr}_3$, a reentrant phase transition allows us to map the strain onto the cuboctahedral void, in terms of the shape of the cuboctahedral void and the organic cation orientation. Our results enable a better understanding of the complex energy landscape of hybrid perovskites, which is essential to building theoretical models to enable technological innovation.

¹This work at Colorado State University was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, under Award SC0016083.

Eve Mozur
Colorado State Univ

Date submitted: 13 Sep 2017

Electronic form version 1.4