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

Octahedral Tilting from Organic Cations in Defect-Ordered Hybrid Perovskites[1] ANNALISE MAUGHAN, Colorado State Univ, ALEX GANOSE, University College London, ANDREW CANDIA, JULIETTE GRANGER, Colorado State Univ, DAVID SCANLON, University College London, JAMES NEILSON, Colorado State Univ — Perovskite semiconductors such as methylammonium lead iodide ($CH_3NH_3PbI_3$) are a technologically-relevant family of materials, finding applications in field-effect transistors, light-emitting diodes, and low-cost photovoltaics, yet materials such as methylammonium lead iodide present significant concerns for toxicity and material stability. Defect-ordered perovskites provide a platform to study optical and electronic behavior in materials with improved toxicity and stability outlooks relative to lead-containing counterparts. We have prepared the series of vacancy-ordered double perovskites A_2SnI_6, where A = Cs^+, $CH_3NH_3^+$, and $CH(NH_2)_2^+$. While Cs_2SnI_6 exhibits moderate electronic conductivity, incorporation of $CH_3NH_3^+$ and $CH(NH_2)_2^+$ reduces carrier mobility across the series. We correlate the observed trends in carrier mobility with rotational disorder and anharmonicity of the [SnI_6] octahedral units, which is enhanced through hydrogen bond formation in the hybrid $(CH_3NH_3)_2SnI_6$ and $(CH(NH_2)_2)_2SnI_6$ compounds. These studies provide an avenue to explore the influence of organic-inorganic coupling on the properties of perovskite-based materials for emerging optical and electronic applications.

[1]This research is supported by the grant DE-SC0016083 funded by the U.S. Department of Energy, Office of Science.

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Date submitted: 19 Sep 2017 Electronic form version 1.4