Octahedral Tilting from Organic Cations in Defect-Ordered Hybrid Perovskites\textsuperscript{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$_3$NH$_3$PbI$_3$) 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 $A_2$SnI$_6$, where $A = $ Cs$^+$, CH$_3$NH$_3^+$, and CH(NH$_2$)$_2^+$. While Cs$_2$SnI$_6$ exhibits moderate electronic conductivity, incorporation of CH$_3$NH$_3^+$ 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$_3$NH$_3$)$_2$SnI$_6$ and (CH(NH$_2$)$_2$)$_2$SnI$_6$ 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.

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