

Abstract Submitted  
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**Hybrid organic-inorganic halide perovskites: Electronic structure, dielectric properties, native defects, and the role of  $ns^2$  ions** MAOHUA DU, Oak Ridge National Laboratory, DONGWEN YANG, College of Materials Science and Engineering, Jilin University, China, HONGLIANG SHI, Oak Ridge National Laboratory, LIJUN ZHANG, College of Materials Science and Engineering, Jilin University, China —  $\text{CH}_3\text{NH}_3\text{PbI}_3$  possesses an interesting combination of properties, i.e., efficient carrier transport, high density of defects (which are nevertheless benign in terms of carrier trapping), large static dielectric constant, and significant ion migration. These properties have important effects on the solar cell performance and are unusual for a photovoltaic material. However, they are not unique; they have been reported for other halides. In the talk, we discuss the underlying physics behind these material properties in  $\text{CH}_3\text{NH}_3\text{PbI}_3$  and other halide electronic materials. The large static dielectric constant resulting from the presence of the  $ns^2$  ions and the molecular dipoles is related to the high defect concentration, defect tolerance, and the defect diffusion. We will also show the calculations of the defect and impurity diffusion and discuss their impact on the solar cell performance.

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