

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Electronic Structure Approach to Tunable Electronic Properties of Hybrid Organic-Inorganic Perovskites GARNETT LIU, Department of Chemistry, Duke University, Durham, NC 27708, WILLIAM HUHN, DAVID B. MITZI, MEMS Department, Duke University, Durham, NC 27708, YOSUKE KANAI, Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC 27599, VOLKER BLUM, MEMS Department, Duke University, Durham, NC 27708 — We present a study of the electronic structure of layered hybrid organic-inorganic perovskite (HOIP) materials using all-electron density-functional theory. Varying the nature of the organic and inorganic layers should enable systematically fine-tuning the carrier properties of each component. Using the HSE06 hybrid density functional including spin-orbit coupling (SOC), we validate the principle of tuning subsystem-specific parts of the electron band structures and densities of states in $\text{CH}_3\text{NH}_3\text{PbX}_3$ ($\text{X}=\text{Cl}, \text{Br}, \text{I}$) compared to a modified organic component in layered $(\text{C}_6\text{H}_5\text{C}_2\text{H}_4\text{NH}_3)_2\text{PbX}_4$ ($\text{X}=\text{Cl}, \text{Br}, \text{I}$) and $\text{C}_{20}\text{H}_{22}\text{S}_4\text{N}_2\text{PbX}_4$ ($\text{X}=\text{Cl}, \text{Br}, \text{I}$). We show that tunable shifts of electronic levels indeed arise by varying $\text{Cl}, \text{Br}, \text{I}$ as the inorganic components, and CH_3NH_3^+ , $\text{C}_6\text{H}_5\text{C}_2\text{H}_4\text{NH}_3^+$, $\text{C}_{20}\text{H}_{22}\text{S}_4\text{N}_2^{2+}$ as the organic components. SOC is found to play an important role in splitting the conduction bands of the HOIP compounds investigated here. The frontier orbitals of the halide shift, increasing the gap, when Cl is substituted for Br and I .

Garnett Liu
Department of Chemistry, Duke University, Durham, NC 27708

Date submitted: 06 Nov 2015

Electronic form version 1.4