

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Atomic-level Design of Water-resistant Hybrid Perovskites with Optimal Band Gap for Solar Cells HONG FANG, PURU JENA, Virginia Commonwealth University — Organic-inorganic hybrid perovskites hold the promise to become the next generation solar-cell materials. However, it is wellknown that these materials, exemplified by $\text{CH}_3\text{NH}_3\text{PbI}_3$, will readily decompose with a trace amount of water under heat, which is perhaps the biggest and the most pressing problem in the field. In this work, we unveil the strategy to make the hybrid perovskites water-proof and also demonstrate the way to control their band gaps at the atomic level. A new family of hybrid perovskites is designed, which are both water-resistant and can achieve the optimal band gap smaller than that of $\text{CH}_3\text{NH}_3\text{PbI}_3$.

Hong Fang
Virginia Commonwealth University

Date submitted: 18 Nov 2016

Electronic form version 1.4