Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Super-ion inspired colorful hybrid perovskite solar cells. HONG FANG, PURU JENA, Virginia Commonwealth Univ — Organic-inorganic hybrid perovskites, with the general formula AMX_3 (A=cation; M=metal; X=halogen), have emerged as a new generation of efficient yet inexpensive photovoltaic cells. These materials show record high conversion efficiency as solar cells and have excellent light-emission properties that can also be used in other optoelectronic devices. They can be processed easily from solution with optic band gaps, tunable from visible to infrared regions and are considered to be "the next big thing in photovoltaics". However, several important issues such as the relationship between their photoexcitation properties and the chemical structures, their stability under ambient conditions, as well as the possibility to invent their environment-friendly analogues remain unsolved. In this work, our aim is not only to gain a fundamental understanding of the structure-property relationship of organic-inorganic hybrid perovskites, but also to rationally design a new class of hybrid perovskites that have desired electronic band gaps for solar cell applications. This is accomplished by using super-ions that can mimic the properties of elementary alkali and halogen ions as building blocks. These super-ions include superalkalis – $CH_3NH_3^+$, $HC(NH_2)_2^+$, and Li_3O^+ as cations and hyperhalogens – $Ge(BH_4)_3^-$ and $Sn(BH_4)_3^-$ as anions. The results are compared with perovskites composed of $GeCl_3^-$, $GeBr_3^-$, GeI_3^-, $SnCl_3^-$, $SnBr_3^-$, and SnI_3^- superhalogen anions. We develop a strategy to assemble these super-ions to form environment-friendly solar cells with adjustable band gaps (covering the visible range and beyond) and with improved resistance to moisture.

Hong Fang
Virginia Commonwealth Univ

Date submitted: 04 Nov 2015 Electronic form version 1.4