Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Ab initio study of the polarization dependence of the optoelectronic properties of hybrid halide perovskites LINN LEPPERT, SEBASTIAN E. REYES-LILLO, Molecular Foundry, Lawrence Berkeley National Lab; Department of Physics, University of California Berkeley, JEFFREY B. NEATON, Molecular Foundry, Lawrence Berkeley National Lab; Department of Physics, University of California Berkeley; Kavli Energy NanoSciences Insitute, NEATON TEAM — With efficiencies as high as 20%, hybrid organic-inorganic halide perovskites have garnered much of the photovoltaic community's attention. In light of recent experimental results [1], we investigate the coupling mechanism between polarization and optoelectronic properties of methylammonium (MA) lead iodide, $(CH_3NH_3)PbI_3$, and related halide perovskites. In particular, we study the conditions that promote a combined effect of strong spin-orbit coupling and inversion symmetry breaking and that lead to a sizable Rashba/Dresselhaus effect. Using density functional theory calculations, we elucidate the emergence of Rashba/Dresselhaus splitting associated with local distortions and long-range coherent alignment of MA moieties in the material. We examine the extent to which the magnitude of the splitting, as well as other important electronic and optical properties [1], can be altered by increasing the macroscopic polarization. This opens avenues for manipulation of optoelectronic properties by an external electric field and/or chemical substitution of the MA molecule.

[1] S.Y. Leblebici, L. Leppert, et al, Facet-dependent photovoltaic efficiency variations in single perovskite grains, submitted (2015).

Linn Leppert
Lawrence Berkeley National Lab

Date submitted: 04 Nov 2015 Electronic form version 1.4