Abstract Submitted
for the TSS17 Meeting of
The American Physical Society

Rashba splitting, spin orbit corrections and their implications in organolead halide perovskites ERIC WELCH, ALEX ZAKHIDOV, LUISA SCOLFARO, None — CH3NH3PbI3 (MAPI) has become a benchmark light harvesting material in emergent, high-efficiency solar applications. It is a strongly absorbing, direct 1.6 eV bandgap, intrinsic semiconductor with balanced carrier mobilities, shallow defect levels, and a >1-micron carrier diffusion length; all important metrics for high performing solar cell absorbers. In this work, first principles modeling is performed on the MAPI structure using density functional theory. Due to the presence of the heavy lead atom, spin orbit coupling (SOC) must be considered when doing *ab-initio* calculations on the material. It has been shown previously that the GGA+U methodology with and without SOC allows to study the formation of polarons (a charge carrier together with its self-induced polarization) in the system.....[1]. Yet, the presence of SOC does qualitatively change the band structure of MAPI, lifting the conduction band degeneracies, and thus resulting in Rashba-type splitting. It can be shown that such spin-texture can lead to ultra-fast polarization dependent photocurrents in the absence of the external bias field. [1]E. Welch, L. Scolfaro, and A. Zakhidov, Density functional theory +u modeling of polarons in organohalide lead perovskites, *AIP Adv.* **6**, 125037 (2016).

Eric Welch
None

Date submitted: 10 Feb 2017 Electronic form version 1.4