Abstract Submitted
for the TSF15 Meeting of
The American Physical Society

DFT and DFT+U Calculations of Lead Halide Perovskites Modeling Polaron Behavior and Doping ERIC WELCH, Texas State Univ-San Marcos, PAUL ERHART, Chalmers University of Technology, LUISA SCOLFARO, ALEX ZAKHIDOV, Texas State Univ-San Marcos — Due to the ever present drive towards improved efficiencies in solar cell technology, new and improved materials are emerging rapidly. One class of materials, organic halide perovskites, are a promising prospect with efficiencies surpassing 20%. This requires a fundamental understanding of the perovskite structures as well as an explanation for physical phenomena. However, explanations of certain physical phenomena, specifically a high recombination rate and low mobility of charge carriers are still controversial. One possible explanation is the formation of self trapped holes, something seen in perovskites like SrTiO3. Methylammonium lead iodide (MAPbI3) and methylammonium lead iodine doped with chlorine ($MAPbI_{-x}Cl_x$) are the perovskites studied in this paper as they are the most promising of the organic halide perovskites. It is shown that a partially localized state is realized using DFT+U calculations. Then, the addition of chlorine is shown to have an effect on the band structure of the MAPbI such that certain crystal directions have greater dispersion (concavity) and thus a larger mobility. It is predicted that a study of the polaron behavior in the chlorine doped molecule will show a similar localized state as the pure MAPbI molecule.

Eric Welch
Texas State Univ-San Marcos

Date submitted: 01 Oct 2015 Electronic form version 1.4