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DFT+U Modeling of Hole Polarons in Organic Lead Halide Perovskites ERIC WELCH, Texas State Univ-San Marcos, PAUL ERHART, Chalmers Institute 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. Organic halide perovskites are a promising prospect, yet a fundamental understanding of the organic perovskite structure and electronic properties is missing. Particularly, explanations of certain physical phenomena, specifically a low recombination rate and high mobility of charge carriers still remain controversial. We theoretically investigate possible formation of hole polarons adopting methodology used for oxide perovskites. The perovskite studied here is the ABX_3 structure, with A being an organic cation, B lead and C a halogen; the combinations studied allow for $A_{1-x}A_{2,1-x}BX_{1,x}X_{2,3-x}$ where the alloy convention is used to show mixtures of the organic cations and/or the halogens. Two organic cations, methylammonium and formamidinium, and three halogens, iodine, chlorine and bromine are studied. Electronic structures and polaron behavior is studied through first principle density functional theory (DFT) calculations using the Vienna Ab Initio Simulation Package (VASP). Local density approximation (LDA) pseudopotentials are used and a +U Hubbard correction of 8 eV is added; this method was shown to work with oxide perovskites. It is shown that a localized state is realized with the Hubbard correction in systems with an electron removed, residing in the band gap of each different structure. Thus, hole polarons are expected to be seen in these perovskites.

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