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**Light-induced defects in hybrid lead halide perovskite** ONISE SHARIA, WILLIAM SCHNEIDER, University of Notre Dame — One of the main challenges facing organohalide perovskites for solar application is stability. Solar cells must last decades to be economically viable alternatives to traditional energy sources. While some causes of instability can be avoided through engineering, light-induced defects can be fundamentally limiting factor for practical application of the material. Light creates large numbers of electron and hole pairs that can contribute to degradation processes. Using *ab initio* theoretical methods, we systematically explore first steps of light induced defect formation in methyl ammonium lead iodide, $MAPbI_3$. In particular, we study charged and neutral Frenkel pair formation involving Pb and I atoms. We find that most of the defects, except negatively charged Pb Frenkel pairs, are reversible, and thus most do not lead to degradation. Negative Pb defects create a mid-gap state and localize the conduction band electron. A minimum energy path study shows that, once the first defect is created, Pb atoms migrate relatively fast. The defects have two detrimental effects on the material. First, they create charge traps below the conduction band. Second, they can lead to degradation of the material by forming Pb clusters.

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