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Light induced polaron formation in perovskite solar cell devices AMANDA NEUKIRCH, WANYI NIE, JEAN-CHRISTOPHE BLANCON, LANL, KANNATASSEN APPAVOO, BNL, HSINHAN TSAI, LANL, MANISH CHHOWALLA, Rutgers University, MUHAMMAD ALAM, Purdue University, MATTHEW SFEIR, BNL, CLAUDINE KATAN, ISCR, JACKY EVEN, FOTON, JARED CROCHET, GAUTUM GUPTA, ADITYA MOHITE, SERGEI TRETIAK, LANL — The need for a low-cost, clean, and abundant source of energy has generated large amounts of research in solution processed solar cell materials. The lead halide perovskite has rapidly developed as a serious candidate for the active layer of photovoltaic devices. The efficiencies of devices made with this material have increased from 3.5% to over 20% in around 5 years. Despite the remarkable progress associated with perovskite materials, there are still fundamental questions regarding their lack of photo-stability over prolonged solar irradiation that need to be addressed. Recent experiments on photo-degradation under constant illumination have found fast self-healing by resting the device in the dark for less than 1 minute. Density functional theory and symmetry analysis show that localized charge states couple to local structural lattice distortions and methyl ammonium quasistatic configurations. Once translational symmetry is lost, additional bonding configurations become symmetry allowed, triggering localized charges in the vicinity over time under constant illumination, thus seeding the formation of macroscopic charged domains and preventing efficient charge extraction. Here we present an in-depth study of polaron formation and binding energy at the atomistic level.

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