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Light-induced defect creation and recombination in organic solar cells

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Prolonged exposure to visible, UV and x-ray radiation induces defects in some organic bulk heterojunction solar cells, and the resulting excess recombination reduces the cell efficiency. Optical transitions characteristic of deep localized electronic states are observed by photocurrent spectroscopy and allows the kinetics of defect creation to be measured. The defect creation rate varies greatly with photon energy and saturates after a long exposure. The states are reversible by annealing to about 100C with thermal activation energy of 1.1-1.3 eV. The results suggest that the defects arise from the recombination-induced dissociation of C-H bonds and the migration of the hydrogen to other sites in the polymer. First-principles calculations show that the resulting under-and over-coordinated carbon atoms are deep traps with properties consistent with the measurements. In the absence of light-induced defects, the dominant recombination process is a transition through localized band tail states, which is reflected in the diode forward bias current-voltage characteristics. The diode ideality factor is temperature dependent and related to the band tail slope.