

How does I₂ Dope MAPbI₃ layers p-type?

Insights from optoelectronic properties

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Abstract

Getting insight in, and ultimately control over electronic doping of halide perovskites may improve tuning of their remarkable optoelectronic properties, reflected in what appear to be low defect densities, and as expressed in various charge transport and optical parameters. These properties determine the remarkable performances of photovoltaic and light-emitting devices. Doping is important for charge transport because it determines the electrical field within the photo-absorber layer, which strongly affects charge collection efficiency. Here we report on intrinsic doping of Methyl-ammonium lead tri-iodide, MAPbI₃, thin films of the types used for solar cells and LEDs, by I₂ vapor at a level that does not affect the optical absorption, and leads to a small (< 20 meV, ~ 9 nm) red-shift in the photoluminescence peak. Doping MAPI layers makes the films ten times more conductive electronically, in the dark, which we show is due to p-type doping because we find their work function to increase by 150 mV. The majority carrier (hole) diffusion length increases upon doping, making the material less ambipolar. Our results are well-explained by I₂-exposure decreasing the density of donor defects, likely iodide vacancies (V_I) or defect complexes, containing V_I. Invoking Iodide interstitials, which are acceptor defects, seems less likely based on calculations of the formation energies of such defects in agreement with a recent report on pressed pellets, rather than polycrystalline thin (0.35 um) films used here.