A dominant positron capture and annihilation at vacancies in MAPbI_3 and CsMAFAPb(I_xBr_$1-x$)_3 layers on PEDOT-PPS/ITO/glass substrates

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Hybrid inorganic-organic halide perovskites attract much attention for their application in optoelectronic devices. However, the performances strongly depend on the quality of the active layers and their capacity to withstand device operation without irreversible damage [1,2]. Light illumination is reported to induce ion migration in HOIPs [3]. Applying a bias in dark in $CH_3NH_3PbI_3$ (MAPbI3) based solar cells also results in ion migration [4]. Dark current measurements give evidence of temperature–dependent charge transport mechanisms in $MAPbI_3$ that are respectively related to electron/hole and ion transport [5]. This questions the existence and/or generation of defects in HOIPs and their role in defect-assisted mechanisms of ion migration under bias and light illumination on photovoltaïc performance.

This work focuses on vacancy-type defects. When in neutral or negatively charged states, such defects capture thermalized positrons in their open volume and give rise to annihilation fingerprints specific to the nature of the vacancy-type defects. Positrons have a most striking reproducible and stable behavior in MAPbI3 and $CsMAFAPb(I_xBr_{1-x})_3$ layers spin coated on PEDOT:PPS/ITO/glass substrates in similar conditions by solution growth process. The annihilation characteristics, e-_e+ annihilating pair momentum distribution and positron lifetime spectra, are consistent with huge native vacancy concentration, $\geq 3*10^{18} cm^{-3}$, that efficiently capture thermalized positrons before their annihilation. An additional noticeable property is that the coverage with a PCBM electron transport layer has little effect on these native vacancies. The positron annihilation lifetime in the vacancies, 334(5) ps, has been also earlier observed in sintered MAPbI3 pellets [6]. The nature of the vacancies and their stability with ageing is discussed.

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