Electronic Supplementary Material (ESI) for Sustainable Energy & Fuels.

Formation, location and beneficial role of PbI_2 in lead halide perovskite solar cells

Tian Du[1,2], Claire H. Burges[1], Jinhyun Kim[2], Jiaqi Zhang[1], James R. Durrant[2] and Martyn A. McLachlan[2]*

[1.] *Department of Materials and Centre for Plastic Electronics, Imperial College London, SW7 2BP*

[2.] *Department of Chemistry and Centre for Plastic Electronics, Imperial College London, SW7 2AZ*

*martyn.mclachlan@imperial.ac.uk

Electronic Suuplementary Information

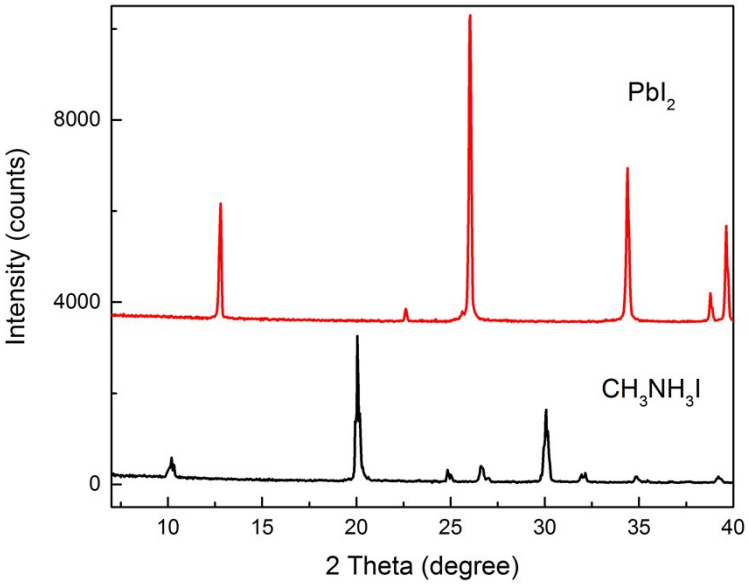

Figure S1 Powder X-ray diffraction patterns of PbI_2 and CH_3NH_3I.

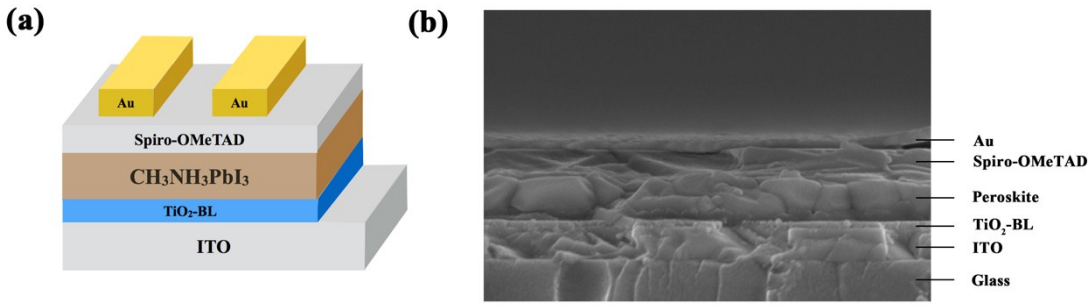

Figure S2 (a) Schematic showing device architecture and (b) the typical cross-sectional SEM image.

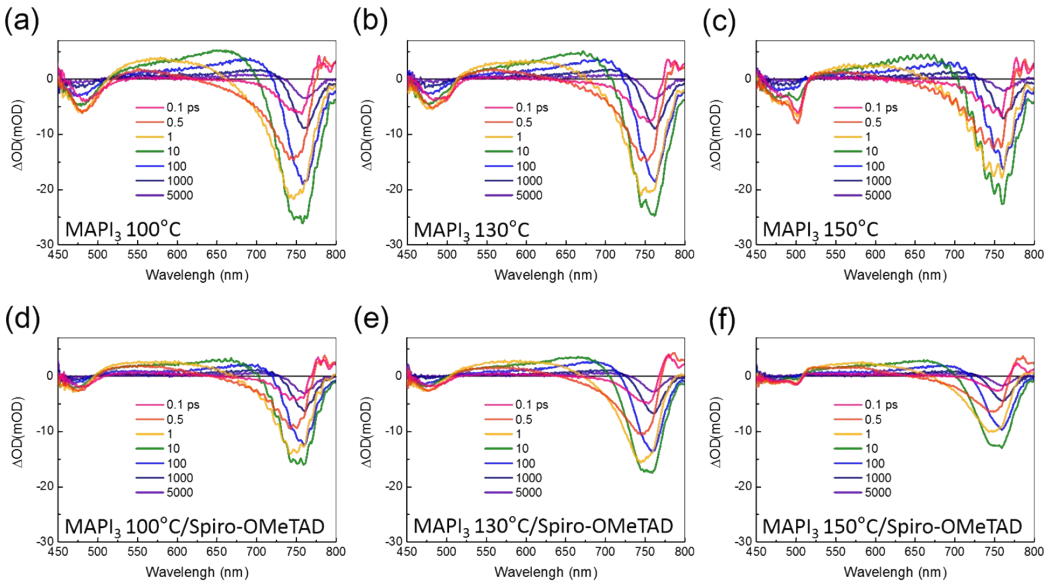

Figure S3 Transient absorption spectrum with excitation at 380nm (flux 64□j/cm2) of MAPI films on glass with (a-c) and without Spiro-OMeTAD quencher (d-e) after being annealed at the indicated temperatures.

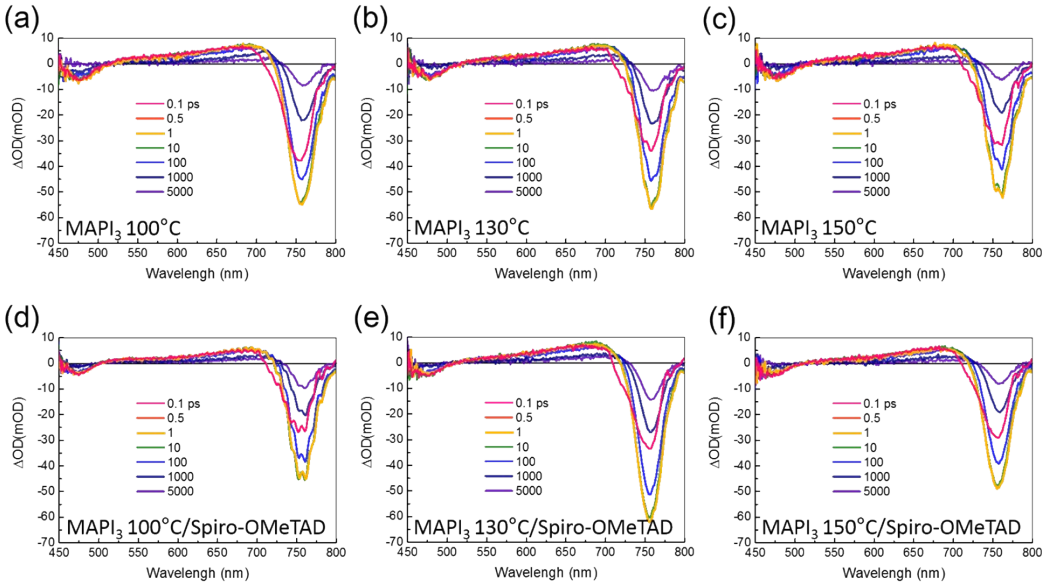

Figure S4 Transient absorption spectrum with excitation at 715 nm (flux 64 □J/cm2) of MAPI films on glass with (a-c) and without Spiro-OMeTAD quencher (d-e) after being annealed at different temperature.

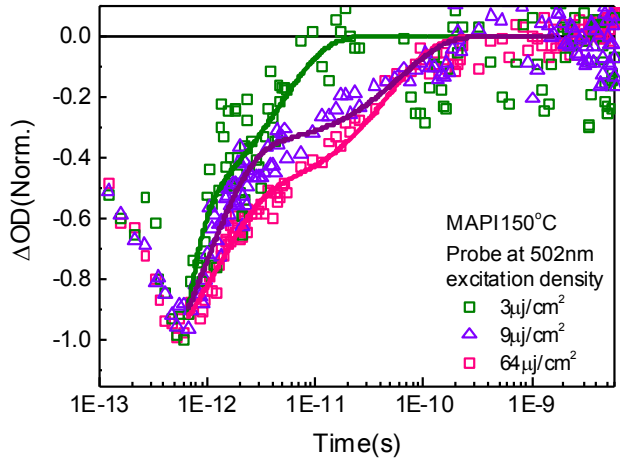

Figure S5 Transient absorption dynamics of 150 °C annealed MAPI films probed at 502 nm, with different excitation density. The symbols are the decays of transient absorption signal, and the solid lines represent double exponential fitting the decays.

Table S1 d-spacings of the lattice planes for MAPI and PbI_2 measured from XRD patterns and calculated from [1]

hkl	Material	$2\theta_{(degrees)}$	$d_{measured}$	$d_{calculated}$
001	PbI_2	12.65	0.6997	0.6979
110	MAPI	14.09	0.6285	0.6258
112	MAPI	20.01	0.4437	0.4450
211	MAPI	23.09	0.3852	0.3778
202	MAPI	24.48	0.3636	0.3627
101	PbI_2	25.39	0.3508	0.3815
220	MAPI	28.43	0.3139	0.3129
310	MAPI	31.84	0.2810	0.2800
003	PbI_2	39.53	0.2280	0.2326

Supporting references

1 N. Onoda-Yamamuro, O. Yamamuro, T. Matsuo and H. Suga, *J. Phys. Chem. Solids*, 1992, **53**, 277–281.