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Enhancing the Stability of Perovskite Solar Cells through Cross-linkable and Hydrogen Bonding Multifunctional Additive

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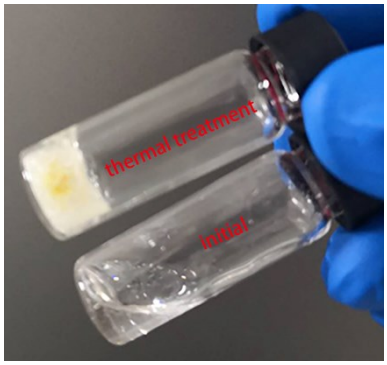

Fig. S1. Photographs of DPPA before and after thermal treatment.

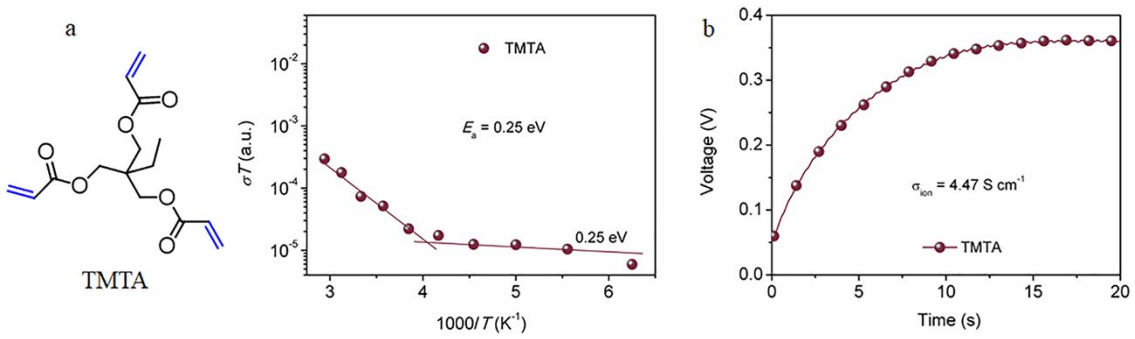

Fig. S2. (a) chemical structure of TMTA additive. (a) activation energy and (b) ions conductivity of perovsktie films with TMTA additive. TMTA additive contains cross-linkable CH2=CH groups (blue), but doesn't contain alkoxy (-O-CH_2) or hydroxyl (-OH) groups.

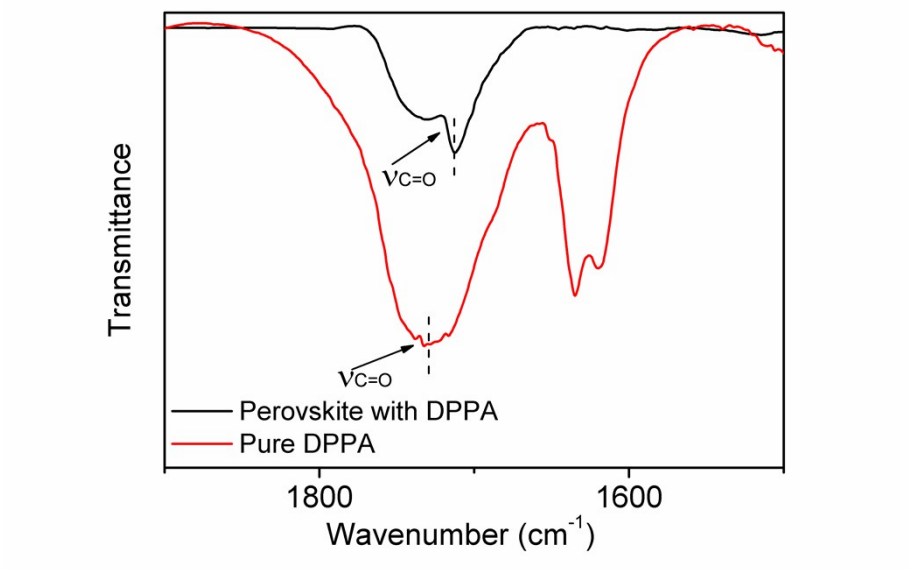

Fig. S3. Enlarged FTIR spectra of pure DPPA and perovskite with DPPA in C=O group region. The shift of $\nu_{C=O}$ can be attributed to the coordination between C=O and PbI_2, which helps to passivate the defects at grain boundaries.

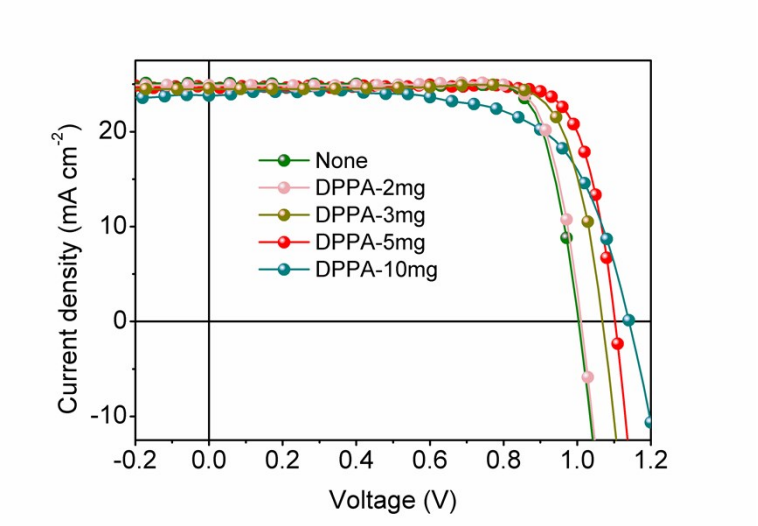

Fig. S4. *J-V* curves of PSCs with different concentration of DPPA.

Table S1. Device parameters of PSCs with different concentration of DPPA.

DPPA concentration (mg mL^{-1})	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF (%)	PCE (%)
0	1.00	25.10	80.5	20.2
2	1.01	24.88	81.7	20.5
3	1.07	24.49	80.9	21.1
5	1.10	24.66	81.0	22.1
10	1.16	23.56	73.4	20.0

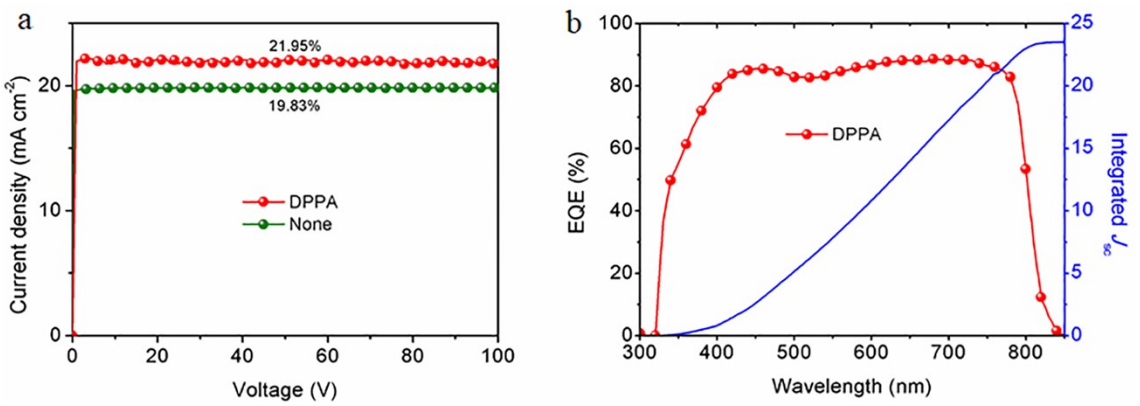

Fig. S5. (a) stabilized maximum power point output and (b) external quantum efficiency (EQE) of PSCs with DPPA.

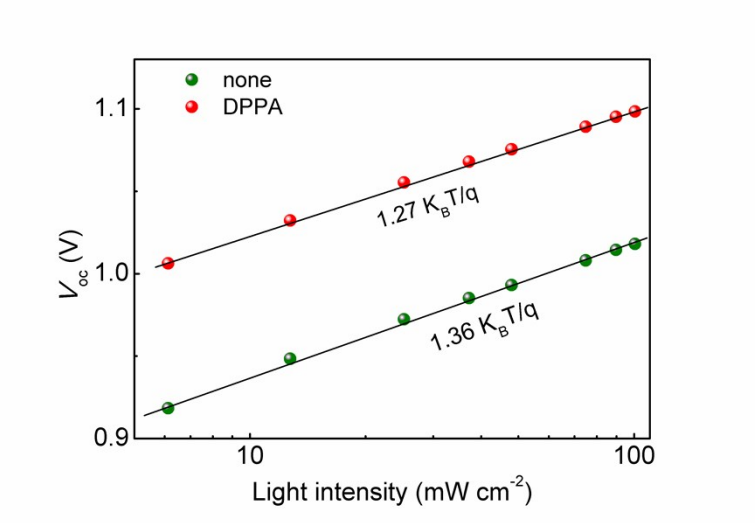

Fig. S6. V_{oc} dependence of PSCs on light intensity.

According to the equation $V_{oc} = V_s + nK_BT/q$ *ln (P/Ps), we can obtain the ideal factor (n) of PSCs, where V_{oc} is the open-circuit voltage, V_s is the voltage under standard sun light, K_B is the Boltzmann constant, T is absolute temperature, q is the elementary charge, P is the light intensity and Ps is one standard sun intensity. Ideally, a device without trapping of charge carriers will exhibit a n-value of 1. When n approaches 2, trap-assisted recombination dominates in the device.

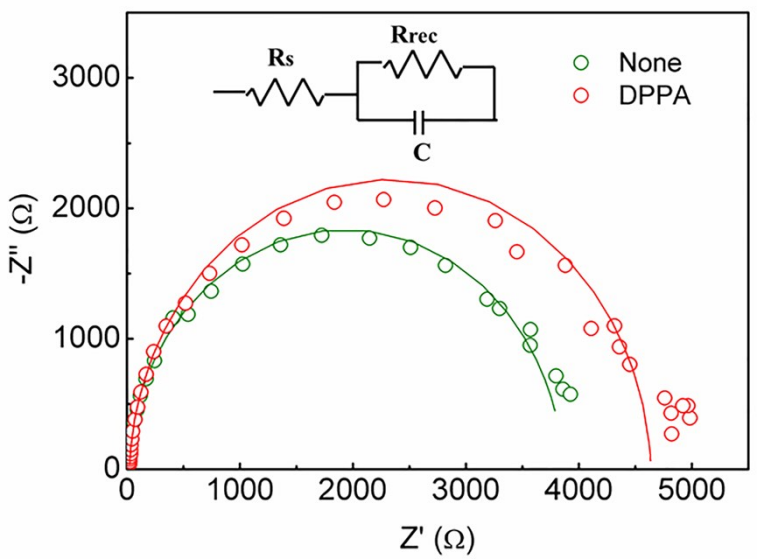

Fig. S7. Electrical impedance spectroscopy (EIS) of PSCs in dark. The inset shows the equivalent circuit in PSCs.

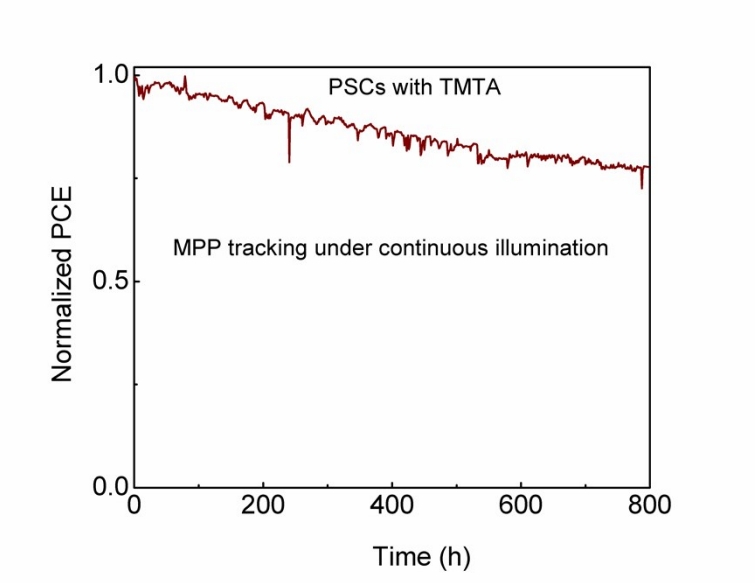

Fig. S8. Operational stability of PSCs with TMTA under MPP tracking conditions.

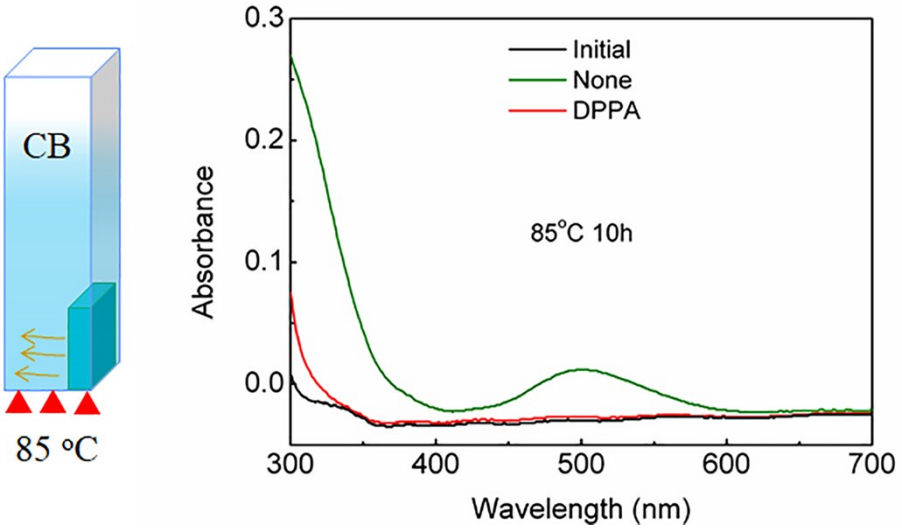

Fig. S9. Immersing experiment of perovskite films in chlorobenzene solvent under 85 °C conditons. In this experiment, Iodine will escape from perovskite layer due to ions diffusion and then transform into I_2, which will be captured by chlorobenzene. The curves show the absorbance of chlorobenzene solvent after immersing perovskite for 10 hours.

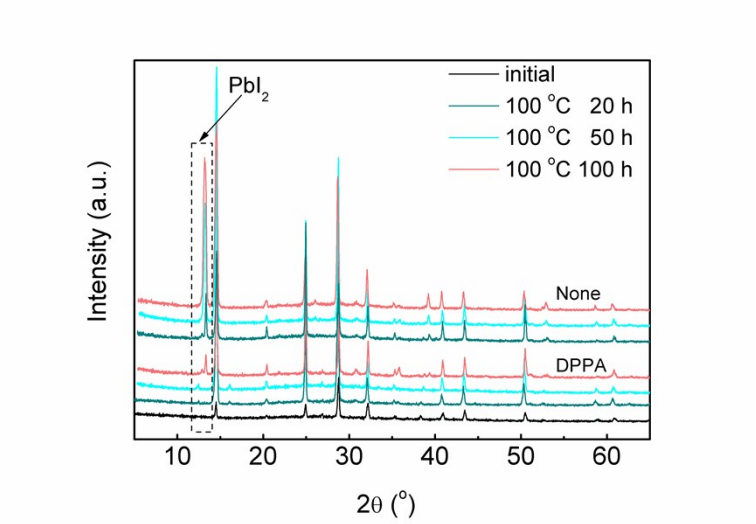

Fig. S10. XRD patterns of perovskite films under thermal conditions (100 °C) for different time.