Supporting Information

Radical Form of PbI_2: A New Defects Passivator for Efficient Perovskite Solar Cells

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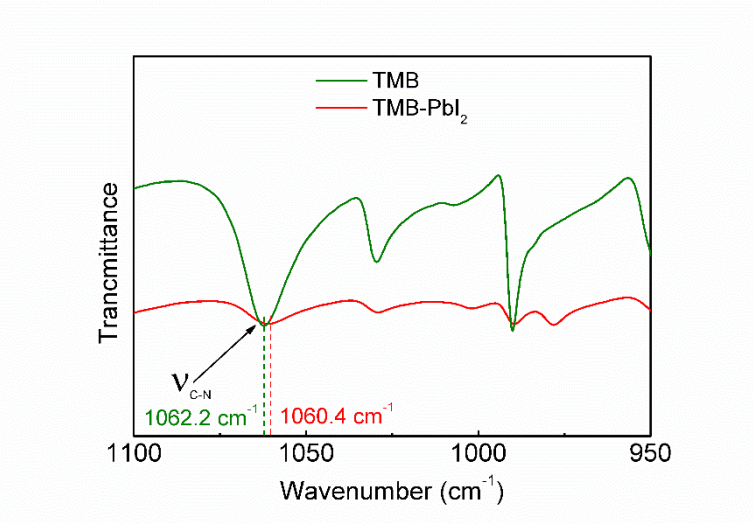


Figure S1. Fourier transform infrared spectra (FTIR) of pure TMB and TMB-PbI_2 radical powder. In TMB-PbI_2, the stretching vibration of C-N bond (C-N) appears at 1060.4 cm^{-1}, which is low-wavenumber shift in comparison with that in TMB (1062.2 cm^{-1}). This result indicates that some chemical interaction exists between TMB and PbI_2.

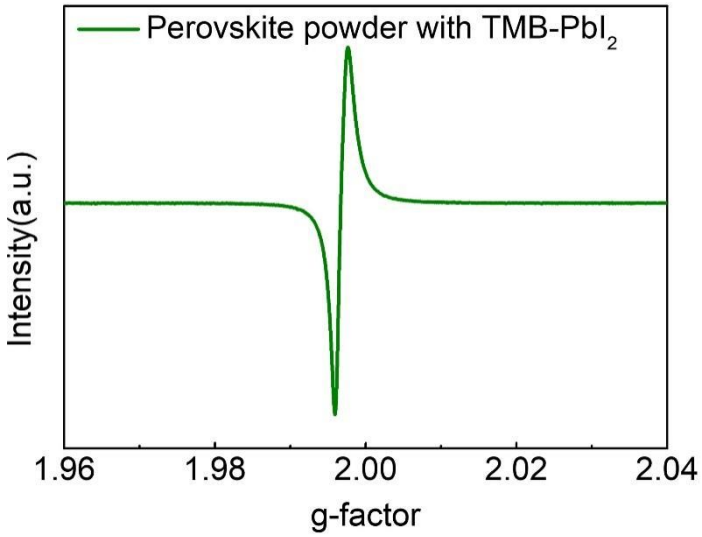


Figure S2. Electron spin resonance (ESR) of perovskite powder with TMB-PbI_2.

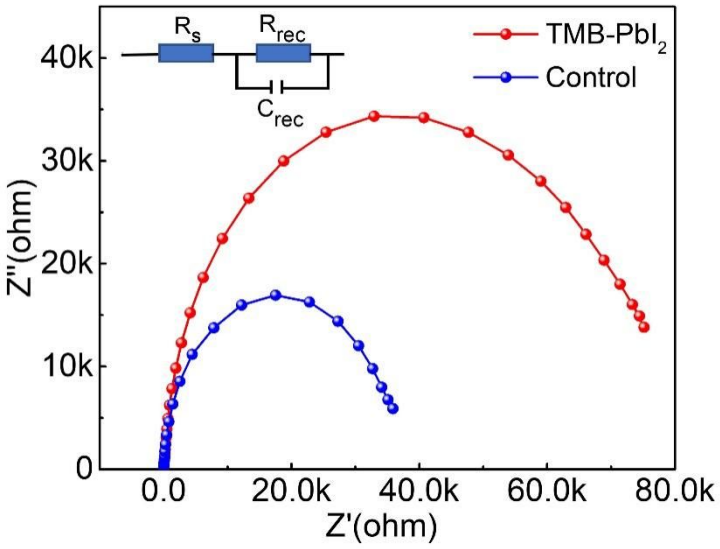


Figure S3. Nyquist plots for the control and TMB-PbI_2 based perovskite devices in the dark.

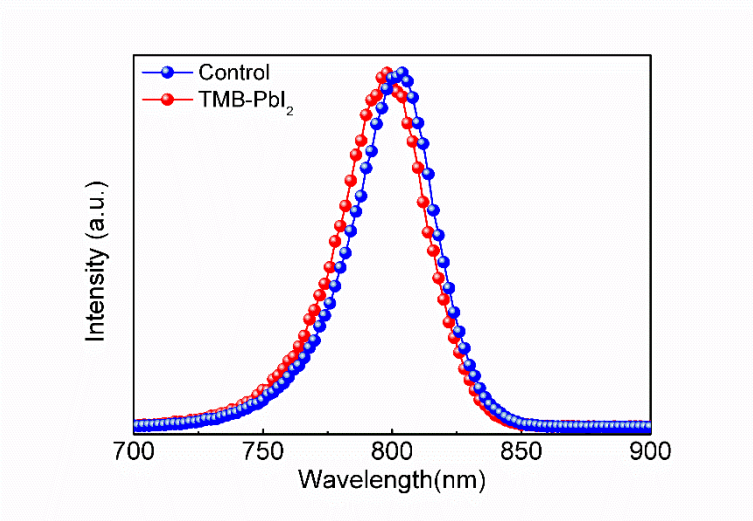
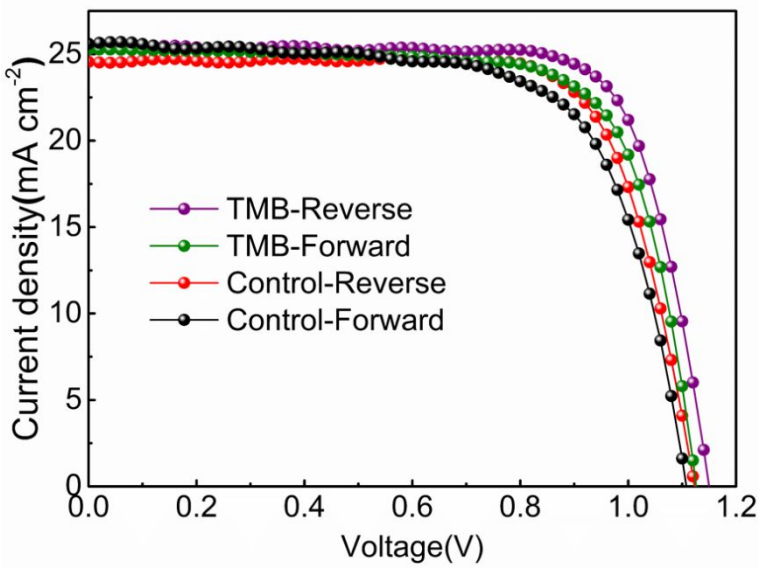
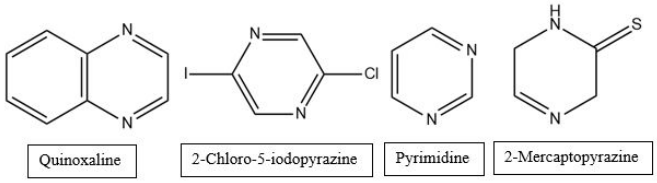


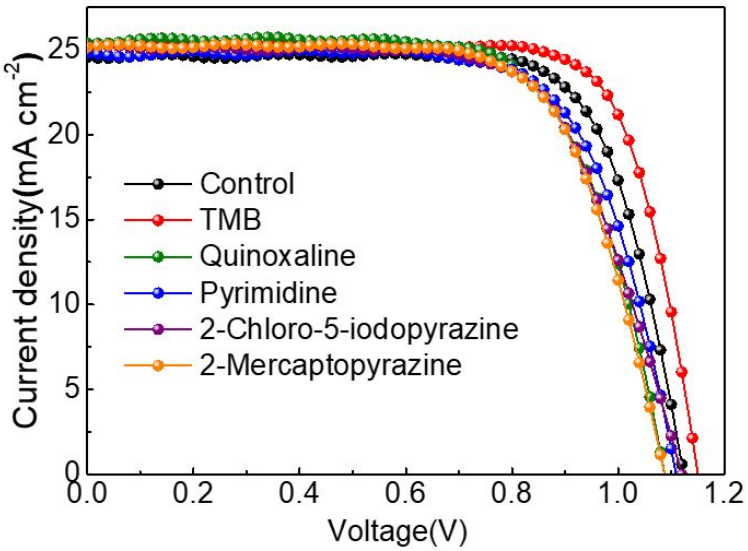
Figure S4. Photoluminescence (PL) spectra of control and TMB-PbI_2 based perovskite films. The films are prepared on a glass substrate. The blue-shift of PL in TMB-PbI_2 based perovskite film indicates the defects passivation.



Name	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF (%)	PCE (%)
TMB-Reverse	1.15	25.71	75.94	22.63
TMB-Forward	1.13	25.32	73.29	20.90
Control-Reverse	1.12	25.40	71.36	20.48
Control- Forward	1.11	25.60	68.55	19.44

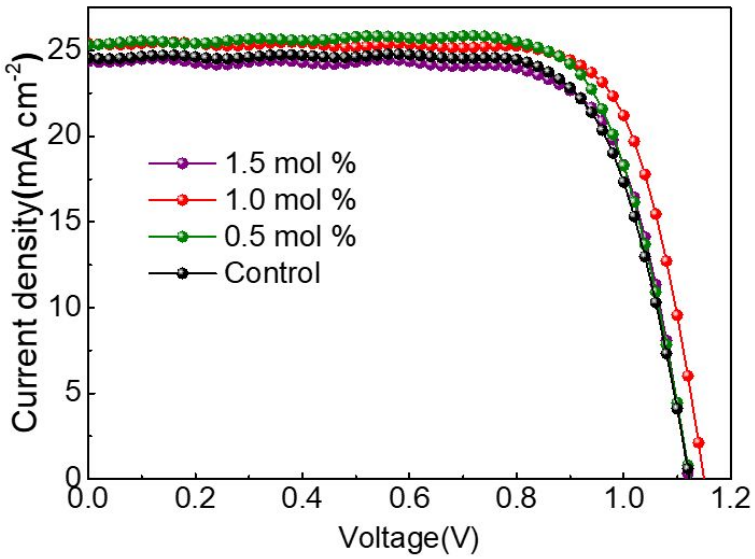
Figure S-5. Comparison of hysteresis between TMB-containing devices and control group devices.





Name	V_{oc} (V)	J_{sc} (mA cm^{-2})	FF (%)	PCE (%)
Control	1.12	25.40	71.36	20.48
TMB-PbI_2	1.15	25.71	75.94	22.63
Quinoxaline	1.11	24.81	70.86	19.71
Pyrimidine	1.12	25.21	68.20	19.25
2-Chloro-5-iodopyrazine	1.09	25.17	70.12	19.20
2-Mercaptopyrazine	1.09	25.42	70.04	19.35

Figure S6. Chemical structure of Nitrogen-containing organic small molecule passivation agent and *J- V* curves and Performance parameter of PSCs under their treatment.



TMB concentration (mol %)	V_{oc} **(V)**	J_{sc} **(mA cm^{-2})**	**FF (%)**	**PCE (%)**
Control	1.12	25.40	71.36	20.48
0.5	1.12	25.33	76.54	21.83
1.0	1.15	25.71	75.94	22.63
1.5	1.12	24.34	74.94	20.68

Figure S7. *J- V* curves of control and different concentration of TMB treatment PSCs.

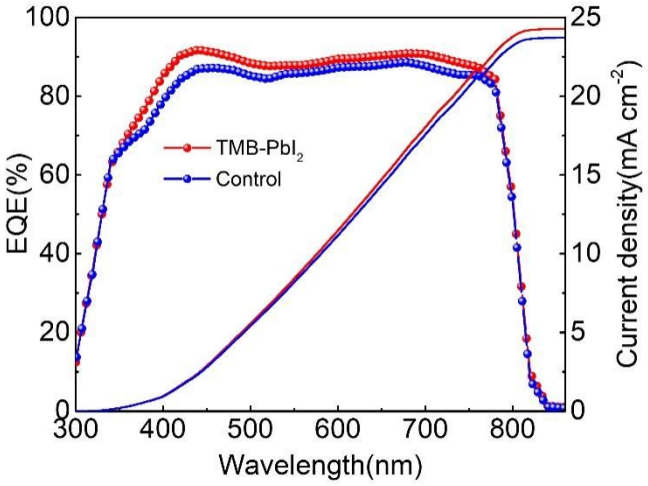


Figure S8. External quantum efficiency (EQE) of control and TMB-PbI_2 based PSCs.

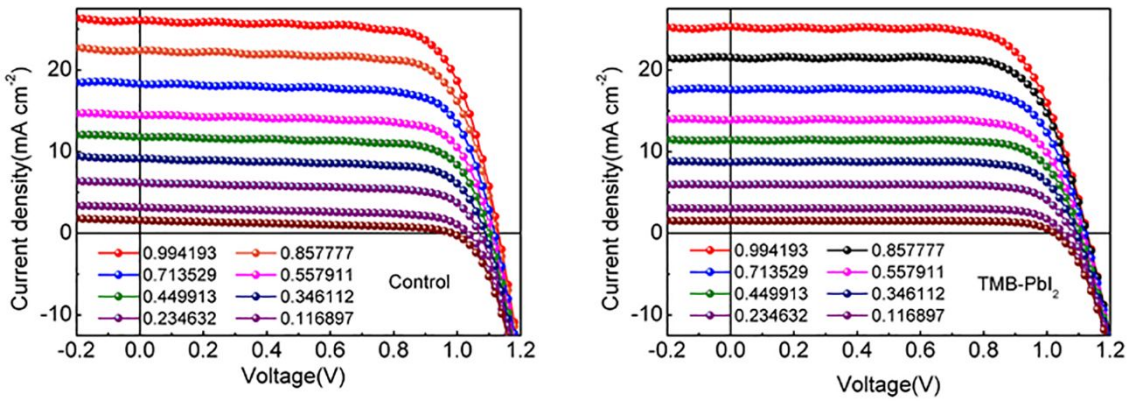


Figure S9. *J-V* curves of control (left) and TMB-PbI_2 (right) based PSCs under different light intensity.

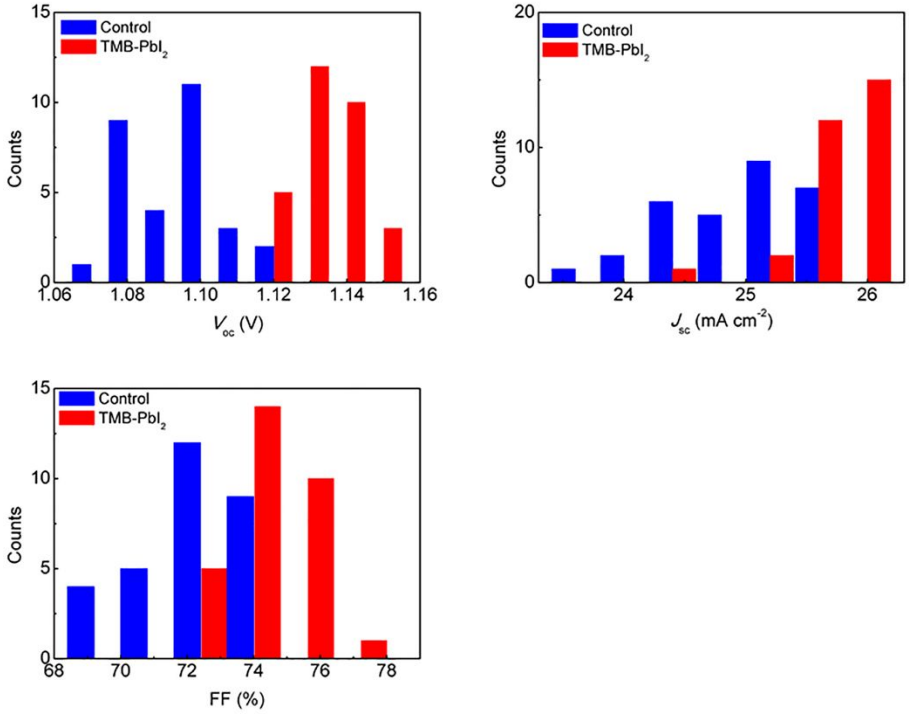


Figure S10. V_{oc}, J_{sc} and FF distribution among 30 separated PSCs.