Electronic Supplementary Information

Enhanced efficacy of defect passivation and charge extraction for efficient perovskite photovoltaics with small open circuit voltage loss

Jin-Feng Liao,^a Wu-Qiang Wu,^{a,b*} Jun-Xing Zhong,^a Yong Jiang,^a Lianzhou Wang,^{b*} and Dai-Bin Kuang^{a*}

^aMOE Key Laboratory of Bioinorganic and Synthetic Chemistry, Lehn Institute of Functional Materials, School of Chemistry, Sun Yat-sen University, Guangzhou 510275, P R China

*Correspondence: <u>wuwuq@mail2.sysu.edu.cn</u>, <u>kuangdb@mail.sysu.edu.cn</u>

^bNanomaterials Centre, School of Chemical Engineering and Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Brisbane, QLD 4072, Australia.

*Correspondence: wuqiang.wu@uq.edu.au, l.wang@uq.edu.au



Fig. S1. The magnified FTIR spectra of pure $g-C_3N_4$, $CH_3NH_3PbI_3$ and $g-C_3N_4$ incorporated $CH_3NH_3PbI_3$ powder scraped from the films deposited on glass substrate.



Fig. S2. XPS spectra of the control $CH_3NH_3PbI_3$ and $g-C_3N_4$ incorporated $CH_3NH_3PbI_3$ films deposited on glass substrate.



Fig. S3. High-resolution TEM image of $g-C_3N_4$ modified $CH_3NH_3PbI_3$ film, showing the heterogeneous anchoring of polymeric $g-C_3N_4$ around the GBs or surface of highly-crystalline perovskite grains.



Fig. S4. Topographic AFM images showing the roughness of the control $CH_3NH_3PbI_3$ and g-C₃N₄ modified $CH_3NH_3PbI_3$ films.



Fig. S5. UV-vis absorption spectra of the of control $CH_3NH_3PbI_3$ and $g-C_3N_4$ incorporated $CH_3NH_3PbI_3$ film deposited on FTO glass substrate.



Fig. S6. PL emission spectra of control $CH_3NH_3PbI_3$ and $g-C_3N_4$ modified $CH_3NH_3PbI_3$ films coated on glass substrate.



Fig. S7. PCEs histogram of a batch of 30 devices based on $g-C_3N_4$ modified $CH_3NH_3PbI_3$ films.



Fig. S8. Top-view SEM image of the $CH_3NH_3PbI_3$ perovskite film incorporated with 0.2 wt% g-C₃N₄.



Fig. S9 Transient photocurrent decay of PSCs incorporated with or without g-C₃N₄.



Fig. S10 The equivalent circuit model used for fitting the Nyquist plots.

Table S1. Summary of the photovoltaic parameters for the PSCs incorporated with different amounts of $g-C_3N_4$ additive.

g-C ₃ N ₄ contents	J _{sc} /mA cm ⁻²	$V_{\rm oc}/V$	η/%	FF
0.05 wt%	22.2	1.12	18.9	0.76
0.1 wt%	23.0	1.16	21.1	0.79
0.2 wt%	21.5	1.08	17.2	0.74
0.1 wt%	23.0	1.16	17.2	0.79

Table S2. The fitted recombination resistance (R_{rec}), capitance (C_2) and the claculated carrier lifetime (τ_e) of the PSCs based on control and g-C₃N₄ modified CH₃NH₃PbI₃ films according to the the Nyquist plots shown in Fig. 5a and 5b.

Bias (V)	$R_{\rm rec}$ (Ω cm ²)		<i>C</i> ₂ (*E ⁻⁸ F)		τ _e (*E ⁻⁴ s)	
	w/o g-	with g-	w/o g-	with g-	w/o g-	with g-
	C_3N_4	C_3N_4	C_3N_4	C_3N_4	C_3N_4	C_3N_4
-0.80	6092	6678	5.47	5.78	3.30	3.90
-0.85	4439	6162	4.72	4.63	2.10	2.90
-0.90	2419	4473	4.02	4.28	0.97	1.90
-0.95	1103	2468	2.93	3.50	0.32	0.86
-1.00	962	1736	2.74	2.85	0.26	0.49

*The carrier lifetime (τ_e) is calculated according to the following equation: $\tau_e = R_{rec} * C_2$.