Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C. This journal is © The Royal Society of Chemistry 2023

Supporting Information for

Trap engineering using oxygen-doped graphitic carbon nitride for high-performance perovskite solar cells

Yaling Lei, ^a Xiaoyan Li, ^a Jingying Liang, ^a Junzhe Shi, ^a Yunhao Wei, ^a Pingli Qin, ^{*b} Hong Tao, ^c Jianjun Chen, ^a Zuojun Tan^{*a} and Hongwei Lei^{*a}

^a College of Science, Huazhong Agricultural University, Wuhan, 430070, China

^b Hubei Key Laboratory of Optical Information and Pattern Recognition, School of Optical Information and Energy Engineering, Wuhan Institute of Technology, Wuhan, 430205, China

^c Hubei Key Laboratory of Plasma Chemistry and Advanced Materials, School of Materials Science and Engineering, Wuhan Institute of Technology, Wuhan 430205, China

Email: leihw@mail.hzau.edu.cn; tzj@mail.hzau.edu.cn; qpl2015@wit.edu.cn



Fig. S1 The preparation process of $g-C_3N_4$ and $g-C_3N_4$ -O.



Fig. S2 The whole survey scan XPS spectra of g-C₃N₄ and g-C₃N₄-O.



Fig. S3 (a) UV-vis transmittance spectra of different ETLs; (b) UV-vis absorption spectra of perovskite film deposited on different ETLs.



Fig. S4 *J-V* curves of MA_{0.7}FA_{0.3}PbI₃ perovskite solar cells with different ETLs(SnO₂ (a),g-SnO₂ (b) and g-O-SnO₂ (c)) under reverse and forward scans.



Fig. S5 Statistic of thePCE(a), Jsc(b), Voc(c) and FF(d) values of PVSCs with different ETLs (SnO₂,g-SnO₂ and g-O-SnO₂).



Fig. S6 I 3d XPS spectra for perovskite films doposited on different ETLs.



Fig. S7 XPS spectra of Sn atoms in different SnO₂.



Fig. S8 The J-V under dark condition on a semi-log plot with different ETLs.



Fig. S9 Steady-state photoluminescence (PL) of perovskite films on different ETLs.



Fig. S10 I-V characteristics of SnO₂, g-SnO₂ and g-O-SnO₂ thin films



Fig. S11 The bandgap diagrams of different electron transport layers(SnO₂, g-SnO₂ and g-O-SnO₂).

Sample	J_{SC} (mA/cm ²)	V _{OC} (V)	Fill Factor (%)	PCE (%)
SnO ₂	23.22	1.05	77.71	18.95
g-SnO ₂	23.08	1.10	77.79	19.75
g-O-SnO ₂	24.44	1.11	77.94	21.14

Table S1. Summary of the photovoltaic performance of devices based on different ETLs.

		1	2	51			
Year	Perovskite(additiv e)	Device Configuration	V _{OC} (V)	J_{SC} (mA cm ⁻²)	FF (%)	PCE (%)	Ref
2017	(FAPbI ₃) _{0.85} (MAP bBr ₃) _{0.15}	FTO/TiO ₂ /TiO ₂ / perovskite/ Spiro-OMeTAD/ Au	1.16	23.18	78	21.3	[1]
2017	$\begin{array}{c} (FA_{0.85}MA_{0.15})_{1-x} \\ Pb(I_{0.85}Br_{0.15})_{3} \\ (KI) \end{array}$	FTO/TiO ₂ :LiMg/TiO ₂ :Li/ perovskite/Spiro-OMeTAD/ Au	1.167	22.99	76	20.32	[2]
2017	(FAPbI ₃) _{0.85} (MAP bBr ₃) _{0.15}	FTO/c-SnO ₂ /(FAPbI ₃) _{0.85} (M APbBr ₃) _{0.15} /spiro-OMeTAD /Au	1.05	22.8	66.2	15.8	[3]
2017	$\begin{array}{l}(FA_{0.85}MA_{0.15})_{0.95}P\\b(I_{0.85}\ Br_{0.15})_3\ (KI)\end{array}$	FTO/SnO ₂ (sol-gel)/ perovskite/Spiro-OMeTAD/ Au	1.132	22.95	79	20.56	[4]
2018	FA _{0.85} MA _{0.15} PbBr _{0.} 45 I _{2.55} (KI)	FTO/TiO2:LiMg/ TiO2:Li/perovskite/Spiro- OMeTAD/Au	1.154	22.92	77.7	20.55	[5]
2018	MAFAPbI _{3-x} Cl _x	FTO/TiO2/perovskite Spiro-OMeTAD/Au	1.04	22.7	75	17.7	[6]
2018	(FAPbI ₃) _{0.85} (MAPbBr ₃) _{0.15}	(FTO)/TiO ₂ /perovskite/ Spiro-OMeTAD/Au	1.07	23.76	80	20.31	[7]
2019	FA _{0.93} MA _{0.07} PbI ₃	ITO/SnO ₂ /Perovskite/ PEAI/Spiro/Au	1.18	25.2	78.4	23.32	[8]
2019	MAxFA _{1-x} PbI _{3-y} Br	$\label{eq:ITO/c-SnO2/MAxFA1-xPbI3-y} \begin{split} ITO/c\text{-}SnO_2/MAxFA_{1\text{-}x}PbI_{3\text{-}y}\\ Br_y + MWCNTc \ /C \end{split}$	1.04	23.5	66.5	16.3	[9]
2019	$\begin{array}{l} FA_{0.83}MA_{0.17}Pb \\ (I_{0.83}Br_{0.17})_3 \ (KI) \end{array}$	FTO/TiOx/perovskite/ Spiro-OMeTAD/Ag	1.15	23.5	75	20.4	[10]
2019	MA:FA:Pb:I:Cl=1: 1:1:3:1	FTO/SnO ₂ /perovskite/ Spiro-OMeTAD /Ag	1.06	23.75	81	20.39	[11]
2020	MAFAPbI ₃ Cl _{3-x}	ITO/SnO ₂ :GQDs/MAFAPbI ₃ Cl _{3-x} /spiro-OMeTAD/Ag	1.11	24.4	0.78	21.1	[12]
2020	MAFAPbI3(TD-N T)	FTO/TiO ₂ /perovskite/Spiro- OMeTAD/Au	1.14	23.85	68.32	19.14	[13]
2021	(FAPbI ₃) _{0.93} MAPb Br ₃) _{0.07}	FTO/TiO ₂ /perovskite/spiro- MeOTAD/Au	1.017	22.196	72.17 6	16.30 1	[14]
2021	FAPbI(47% MAI)	ITO/MeO-2PACz perovskite/C ₆₀ /BCP/Cu	1.05	25.70	75.91	20.4	[15]
2021	(FAPbI ₃) _{0.95} (MAP bBr ₃) _{0.05} (5%HACL)	(FTO)/NiO/perovskite/Spiro- OMeTAD/Au	1.11	24.75	81.03	22.32	[16]
2022	(MA _{0.5} FA _{0.5})PbI ₃ (TAA)	FTO/c-TiO ₂ /mp-TiO ₂ /perovs kite/spiro-MeOTAD/Au	1.109	24.62	78	21.29	[17]
2022	MAFAPbI _{3-x} Cl _x	ITO/SnO ₂ /	1.05	20.94	74.08	16.26	[18]

Table S2. Statistics on the photoelectric conversion efficiency of binary perovskite solar cells.

Year	Perovskite(additiv e)	Device Configuration	<i>V_{OC}</i> (V)	J _{SC} (mA cm ⁻²)	FF (%)	PCE (%)	Ref
		perovskite/P3HT/Au					
2022		FTO/TiO ₂ /ZnO/perovskite/	0.99	21.2	0.67	14.1	[10]
2022	MAXFA1-XP013	Spiro-OMeTAD /MoO ₃ /Ag					[19]
2022	MA _{0.7} FA _{0.3} PbI ₃	FTO/SnO ₂ /perovskite/	1.11	24.44	77.94	21.14	our
		Spiro-OMeTAD/Ag					work

Table S3. The specific numerical value of the Sn atom in SnO₂ XPS spectrum.

		Position	Area	Ration	Sn^{4+}/sn^{2+}
	Sn	484.08	14264	0.022088	
G-SnO ₂	Sn^{4+}	485.88	588515	0.911334	13.69
	Sn^{2+}	487.28	42994	0.066578	
	Sn	483.88	16452	0.022681	
G-O-SnO ₂	Sn^{4+}	485.88	679125	0.936237	22.79
	Sn^{2+}	487.28	29799	0.041082	

Table S4. TRPL decay-time fitting for perovskite films deposited on different electron transport

layers.						
Sample	τ_1 (ns)	A1 (%)	τ_2 (ns)	A2 (%)	$\tau_{average} (ns)$	
PVK+SnO ₂	46.8165	42.90	194.3809	57.10	171.77	
PVK+g-SnO ₂	42.5370	52.34	96.3990	47.66	78.82	
PVK+g-O-SnO ₂	35.3823	37.26	127.4703	62.74	114.44	

Table S5. The energy data of SnO_2 , g- SnO_2 and g-O- SnO_2 from UPS measurements

Sample	E _{cutoff} (eV)	W _F (eV)	E _F (eV)	E _{VBM} (eV)	E _{CBM} (eV)
SnO ₂	17.19	4.01	-4.01	-7.73	-3.89
g-SnO ₂	17.25	3.95	-3.95	-7.71	-3.87
g-O-SnO ₂	17.51	3.69	-3.69	-7.49	-3.65

Work function (W_F) is evaluated by the formula: $W_F = hv - E_{cutoff}$

Fermi level energy (E_F) is evaluated by the formula: $E_F = -W_F$

hv is the photon energy of irradiation light. (21.2 eV)

Valence band energy level (E_{VBM}) is evaluated by the formula: $E_{VBM} = E_F - E_g$

Reference:

- 1 K.T. Cho, S. Paek, G. Grancini, C. Roldán-Carmona, P. Gao, Y. Lee, M.K. Nazeeruddin, *Energy Environ. Sci.*, 2017, 10, 621-627.
- 2 Z. Tang, T. Bessho, F. Awai, T. Kinoshita, M.M. Maitani, R. Jono, T.N. Murakami, H. Wang, T. Kubo, S. Uchida, *Sci. Rep.*, 2017, 7, 1-7.
- P. Pinpithak, H.-W. Chen, A. Kulkarni, Y. Sanehira, M. Ikegami, T. Miyasaka, *Chem. Lett.*, 2017, 46, 382-384.
- 4 T. Bu, X. Liu, Y. Zhou, J. Yi, X. Huang, L. Luo, J. Xiao, Z. Ku, Y. Peng, F. Huang, *Energy Environ. Sci.*, 2017, **10**, 2509-2515.
- 5 Z. Tang, S. Uchida, T. Bessho, T. Kinoshita, H. Wang, F. Awai, R. Jono, M.M. Maitani, J. Nakazaki, T. Kubo, *Nano Energy*, 2018, **45**, 184-192.
- 6 M.M. Tavakoli, P. Yadav, D. Prochowicz, R. Tavakoli, M. Saliba, J. Phys. D., 2018, 52, 034005.
- 7 D. Liu, W. Zhou, H. Tang, P. Fu, Z. Ning, Sci. China Chem., 2018, 61, 1278-1284.
- 8 Q. Jiang, Y. Zhao, X. Zhang, X. Yang, Y. Chen, Z. Chu, Q. Ye, X. Li, Z. Yin, J. You, *Nat. Photonics*, 2019, **13**, 460-466.
- 9 J. Zhou, J. Wu, N. Li, X. Li, Y.-Z. Zheng, X. Tao, J. Mater. Chem. A, 2019, 7, 17594-17603.
- L. Kuai, Y. Wang, Z. Zhang, Y. Yang, Y. Qin, T. Wu, Y. Li, Y. Li, T. Song, X. Gao, Sol. RRL, 2019, 3, 1900053.
- 11 T. Zhang, Q. Xu, F. Xu, Y. Fu, Y. Wang, Y. Yan, L. Zhang, Y. Zhao, *Sci. Bull.*, 2019, 64, 1608-1616.
- 12 S. Pang, C. Zhang, H. Zhang, H. Dong, D. Chen, W. Zhu, H. Xi, J. Chang, Z. Lin, J. Zhang, *Appl. Surf. Sci.*, 2020, **507**, 145099.
- 13 A.M. Elseman, A.H. Zaki, A.E. Shalan, M.M. Rashad, Q.L. Song, *Ind. Eng. Chem. Res.*, 2020, 59, 18549-18557.
- 14 S.H. Joo, H.W. Choi, Coatings, 2021, 11, 1184.
- 15 M. Roß, S. Severin, M.B. Stutz, P. Wagner, H. Köbler, M. Favin-Lévêque, A. Al-Ashouri, P. Korb, P. Tockhorn, A. Abate, *Adv. Energy Mater.*, 2021, **11**, 2101460.
- 16 L. Wang, X. Wang, L. Zhu, S.-B. Leng, J. Liang, Y. Zheng, Z. Zhang, Z. Zhang, X.X. Liu, F. Liu, *Chem. Eng. J.*, 2022, 430, 132730.
- 17 J.V. Patil, S.S. Mali, C.K. Hong, Mater. Today Chem., 2022, 25, 100950.
- 18 G. Wu, X. Dong, G. Cui, R. Sun, X. Wu, M. Gu, Z. Zuo, Y. Liu, Sol. Energy, 2022, 237, 153-160.
- 19 Z. Irshad, M. Adnan, J.K. Lee, J. Mater. Sci., 2022, 57, 1936-1946.