

## Electronic Supplementary Information

# Enhanced performance and stability of low-bandgap mixed lead-tin halide perovskite photovoltaic solar cells and photodetectors *via* defect passivation with UiO-66-NH<sub>2</sub> metal-organic frameworks and interfacial engineering

Chih-Yu Chang,<sup>a</sup> Kuan-Hsi Wu,<sup>a</sup> Chun-Ya Chang,<sup>a</sup> Rui-Fang Guo,<sup>b</sup> Guan-Lin Li,<sup>b</sup> and Cheng-Yu Wang\*<sup>b</sup>

<sup>a</sup> Department of Materials Science and Engineering, National Taiwan University of Science and Technology, Taipei, 10607, Taiwan (R.O.C.).

<sup>b</sup> Department of Materials Science and Engineering, National Yang Ming Chiao Tung University, Hsinchu 30010, Taiwan (R.O.C.). (E-mail: [ChengYuWang@nycu.edu.tw](mailto:ChengYuWang@nycu.edu.tw))

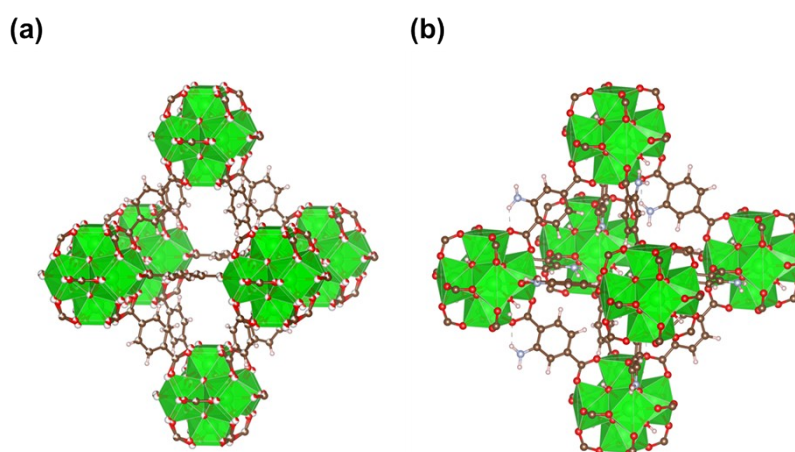
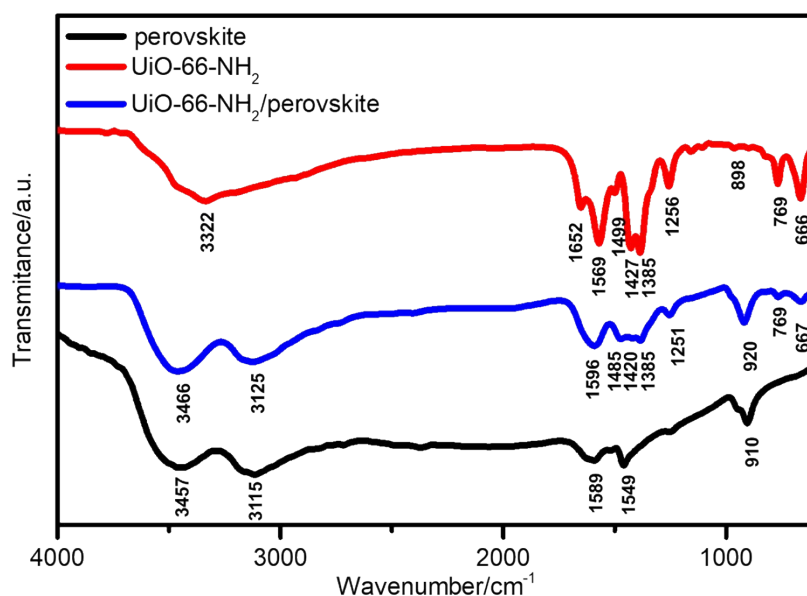
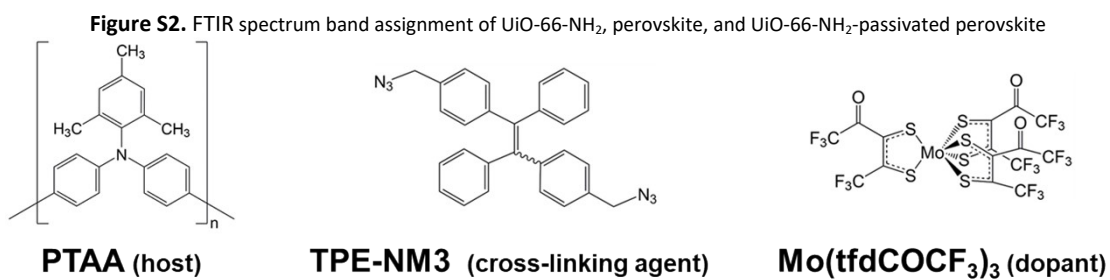
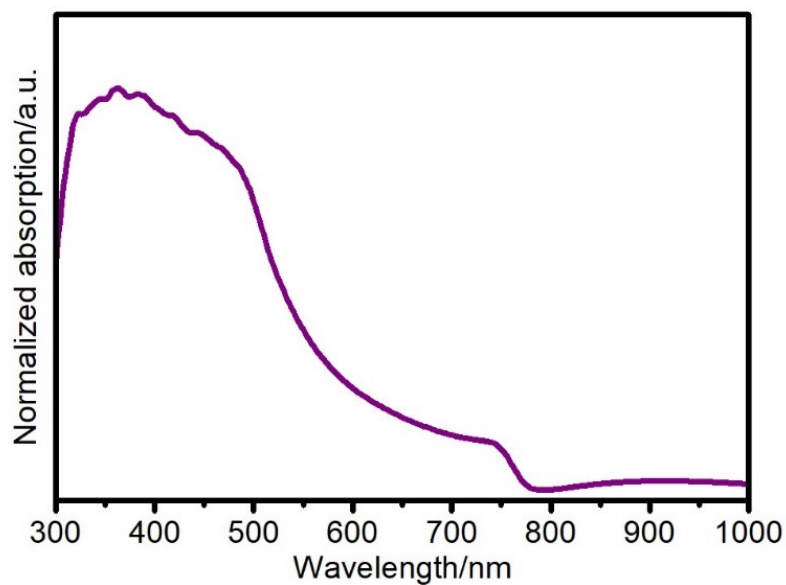


Fig. S1 (a) UiO-66 (ccdc: 733458); (b) UiO-66-NH<sub>2</sub> (ccdc: 1405751)

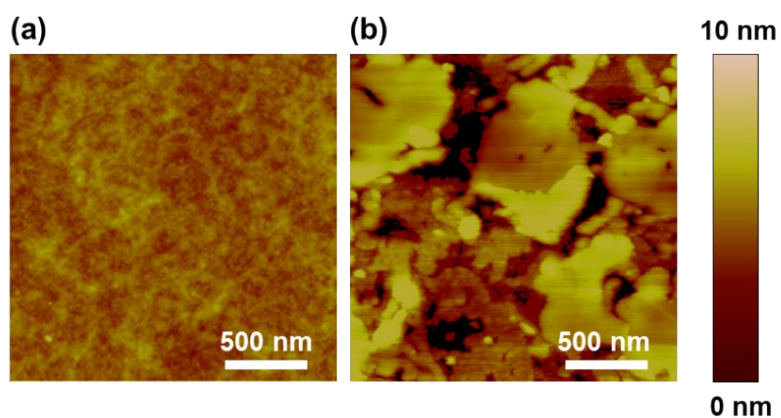




**Fig. S3** Schematic illustration of the molecular structures used in this study.



**Figure S4.** The absorption spectrum of the as-fabricated device



**Fig. S5** AFM topographic images of ITIC films at varied dopant concentrations: (a) 10 mol%. (b) 20 mol%.

**Table S1.** Summary of the photovoltaic performance of MOF-derived PSCs discussed in the text. <sup>1-7</sup>

Reference	MOF and MOF-derived material	Function	Perovskite	Application	Device stability
1	ZIF-8/TiO <sub>2</sub>	ETL	MAPbI <sub>3</sub>	Solar cell	Not reported
2	MZnO	ETL	FA <sub>0.83</sub> CS <sub>0.17</sub> PbI <sub>2.5</sub> Br <sub>0.5</sub>	Solar cell	77% of initial PCE remains after 30 day
3	SP-MOF	HTL	MAPbI <sub>3</sub>	Solar cell	54% of initial PCE remains after 9 day
4	2D graphite NPC	HTL	CS <sub>0.05</sub> FA <sub>0.81</sub> MA <sub>0.14</sub> PbI <sub>2.55</sub> Br <sub>0.45</sub>	Solar cell	85.7% of initial PCE remains after 30 day
5	MOF-808	Interlayer/additive	MAPbI <sub>3</sub>	Solar cell	80% of initial PCE remains after 30 day
5	UiO-66	Interlayer/additive	MAPbI <sub>3</sub>	Solar cell	70% of initial PCE remains after 30 day
6	In <sub>2</sub>	Additive	MAPbI <sub>3</sub>	Solar cell	90% of initial PCE remains after 25 day
7	In-BTC	Additive	CS <sub>0.05</sub> FA <sub>0.81</sub> MA <sub>0.14</sub> PbI <sub>2.55</sub> Br <sub>0.45</sub>	Solar cell	81.3% of initial PCE remains after 12 day
This work	UiO-66-NH <sub>2</sub>	Additive	CH <sub>3</sub> NH <sub>3</sub> Sn <sub>0.25</sub> Pb <sub>0.75</sub> I <sub>3</sub>	Solar cell/PDs	60% of initial PCE remains after 23 day

**Table S2.** List of FTIR band assignment of UiO-66-NH<sub>2</sub>, perovskite, and UiO-66-NH<sub>2</sub>/perovskite

Vibration mode assignment	UiO-66-NH <sub>2</sub> [cm <sup>-1</sup> ]	Perovskite [cm <sup>-1</sup> ]	UiO-66-NH <sub>2</sub> /perovskite [cm <sup>-1</sup> ]
N-H (stretch)		3457	3466
O-H (stretch)	3322		
C-H (stretch)	-	3115	3125
N-H (bending)	1652	1589	1596
O-C-O (asymmetric)	1569	-	1596
C-H (bending)	1499	1459	1485
C=C (aromatic C=C)	1427	-	1420
O-C-O (symmetric)	1385		1385
C-N (stretch)	1256	-	1251
N-H (wag)	898	910	920
Zr-O	769	-	769
Zr-O	666	-	667

**Table S3.** Degradation table of the devices as a function of storage time in ambient conditions (25 °C and 70% relative humidity). Average and standard deviation values are obtained based on 5 devices. The values in parenthesis are for the best-performing devices.

Device A	Storage times [hour]	PCE [%]	Device D	Storage times [hour]	PCE [%]
	0	9.20 ± 0.67 (9.95)		0	13.06 ± 0.76 (13.93)
	14	7.91 ± 0.58 (8.56)		13	11.62 ± 0.67 (12.39)
	65	7.30 ± 0.53 (7.89)		59	10.88 ± 0.63 (11.56)
	123	6.52 ± 0.47 (7.05)		113	10.56 ± 0.61 (10.83)
	184	5.75 ± 0.42 (6.21)		174	9.71 ± 0.56 (10.37)
	277	3.89 ± 0.28 (4.20)		267	9.42 ± 0.55 (10.06)
	391	2.28 ± 0.16 (2.47)		372	8.85 ± 0.52 (9.43)
				454	8.27 ± 0.49 (8.81)
				551	7.87 ± 0.47 (8.40)

## Notes and references

- H.-Y. Chung, C.-H. Lin, S. Prabu and H.-W. Wang, *Journal of the Chinese Chemical Society*, 2018, **65**, 1476-1481.
- Y.-N. Zhang, B. Li, L. Fu, Q. Li and L.-W. Yin, *Electrochimica Acta*, 2020, **330**, 135280.
- L. Huang, X. Zhou, R. Wu, C. Shi, R. Xue, J. Zou, C. Xu, J. Zhao and W. Zeng, *Journal of Power Sources*, 2019, **433**, 226699.
- X. Zhou, L. Qiu, R. Fan, A. Wang, H. Ye, C. Tian, S. Hao and Y. Yang, *Solar RRL*, 2020, **4**, 1900380.
- C.-C. Lee, C.-I. Chen, Y.-T. Liao, K. C.-W. Wu and C.-C. Chueh, *Adv. Sci.*, 2019, **6**, 1801715.
- M. Li, D. Xia, A. Jiang, X. Du, X. Fan, L. Qiu, P. Wang, R. Fan and Y. Yang, *Energy Technol.*, 2019, **7**, 1900027.
- X. Zhou, L. Qiu, R. Fan, J. Zhang, S. Hao and Y. Yang, *Nano-Micro Letters*, 2020, **12**, 80.