

# **Tailoring Lattice Chlorine in Perovskite through Dual-Additive Engineering for Enhanced Photovoltaic Performance**

Dun Ma, Jingwen He, Jie Sheng, Wu Shao, Zhihao Deng, Ronghao Cen,  
Yufei Fu, Wenjun Wu\*

Key Laboratory for Advanced Materials and Institute of Fine Chemicals Shanghai, Key Laboratory of Functional Materials, Chemistry School of Chemistry and Molecular Engineering, East China University of Science and Technology, Shanghai, 200237, China

E-mail: [wjwu@ecust.edu.cn](mailto:wjwu@ecust.edu.cn)

Table S1: Ion chromatographic raw data and its Cl<sup>-</sup> content calculation

	FTO+					
	FTO (mg)	Perovskite (mg)	Perovskite (mg)	IC (mg/L)	Cl <sup>-</sup> (mg)	Cl <sup>-</sup> (%)
40% MACl	814.40	815.30	0.90	1.14	0.03	3.17
20% MACl	814.70	815.60	0.90	0.56	0.01	1.56
20% DMACl	818.90	819.80	0.90	0.39	0.01	1.08
Hybrid	820.60	821.40	0.80	0.34	0.01	1.06

Table S2: Perovskite lattice spacing calculation

	TiO <sub>2</sub>		ZrO <sub>2</sub>	
	2θ/°	d/Å	2θ/°	d/Å
Control	14.09	1.12	14.12	1.10
40% MACl	14.12	1.10	14.13	1.09
20% MACl	14.12	1.10	14.11	1.10
20% DMACl	14.02	1.16	14.02	1.16
Hybrid	14.07	1.13	14.06	1.13

Table S3: TRPL lifetime fitting calculations

	A <sub>1</sub>	τ <sub>1</sub> /ns	A <sub>2</sub>	τ <sub>2</sub> /ns	τ <sub>ave</sub> /ns
Control	4573.38	4.44	0.71	106.63	4.82
40% MACl	165.91	7.48	0.29	126.10	10.86
20% MACl	88.26	8.27	0.35	118.69	14.19
20% DMACl	1780.86	5.08	0.23	170.96	5.79
Hybrid	6509.35	4.35	0.24	164.18	4.57

Table S4: Carrier mobility and diffusion length

	Mobility (10 <sup>-6</sup> m <sup>2</sup> Vs)	Diffusion length (nm)
Control	1.21	12.29
40% MACl	0.95	11.97
20% MACl	1.06	16.70
20% DMACl	1.10	17.52
Hybrid	1.42	23.07

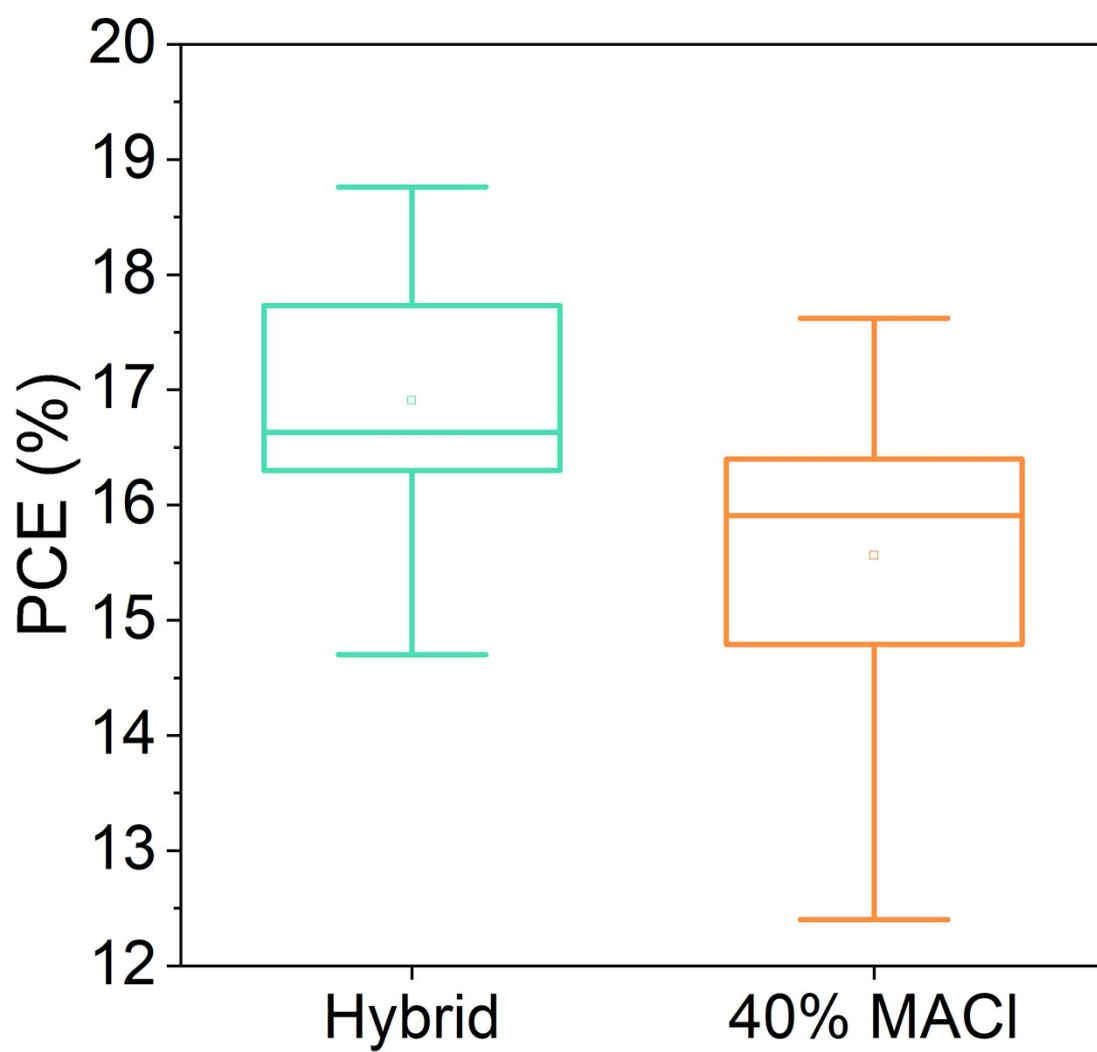


Figure S1: Distribution of photoelectric conversion efficiency for Hybrid and 40% MACl groups

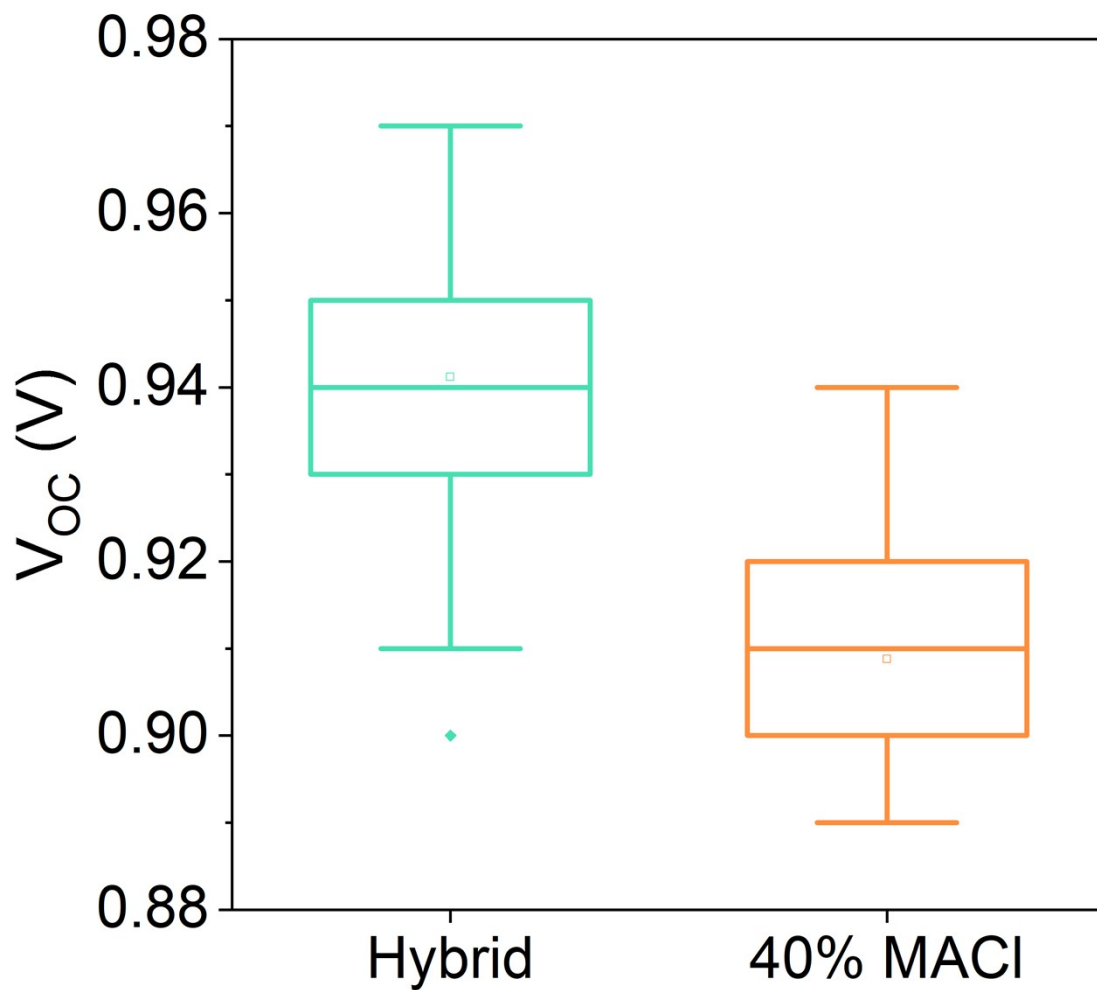


Figure S2: Open-circuit voltage distribution for Hybrid and 40 per cent MACl groups

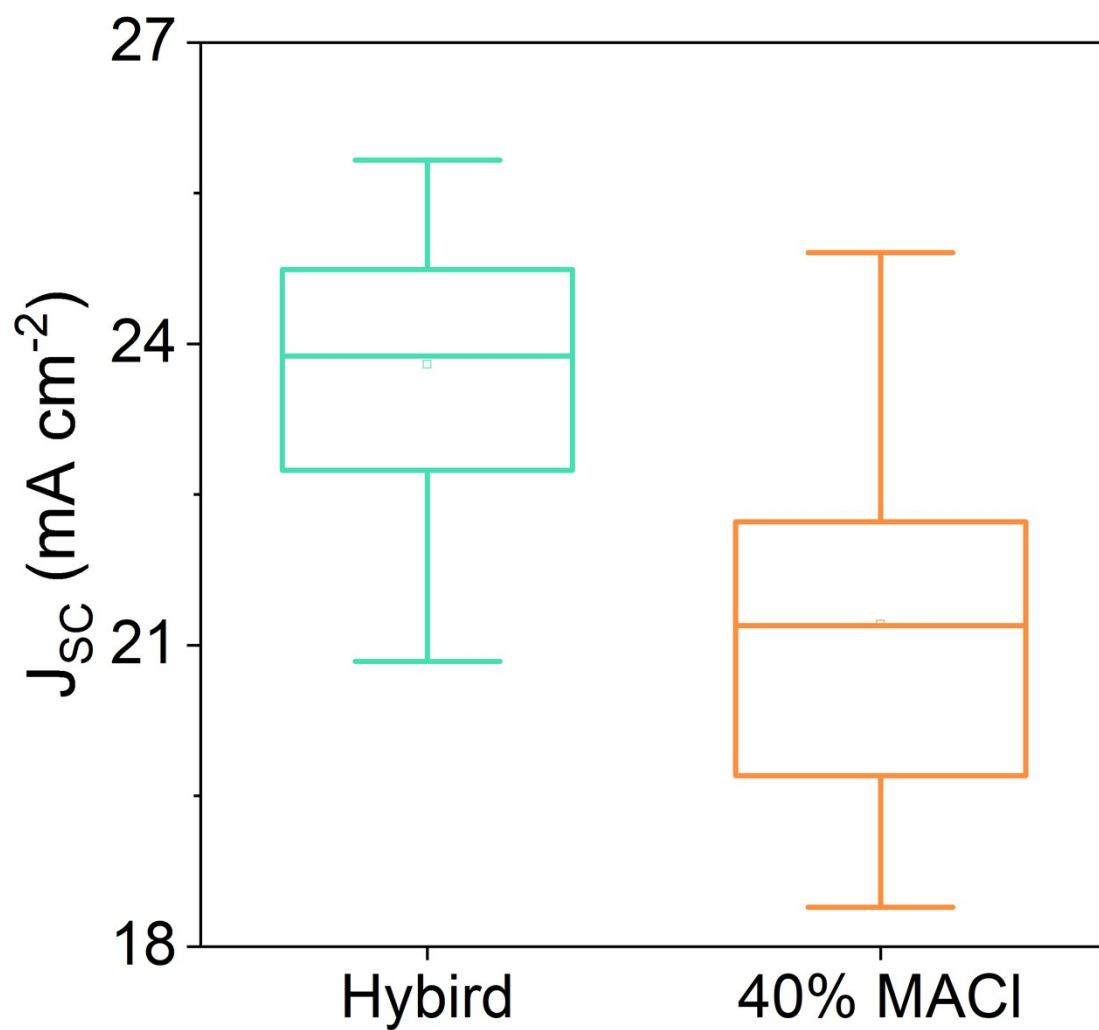


Figure S3: Distribution of short-circuit current density for Hybrid and 40 per cent MACI groups

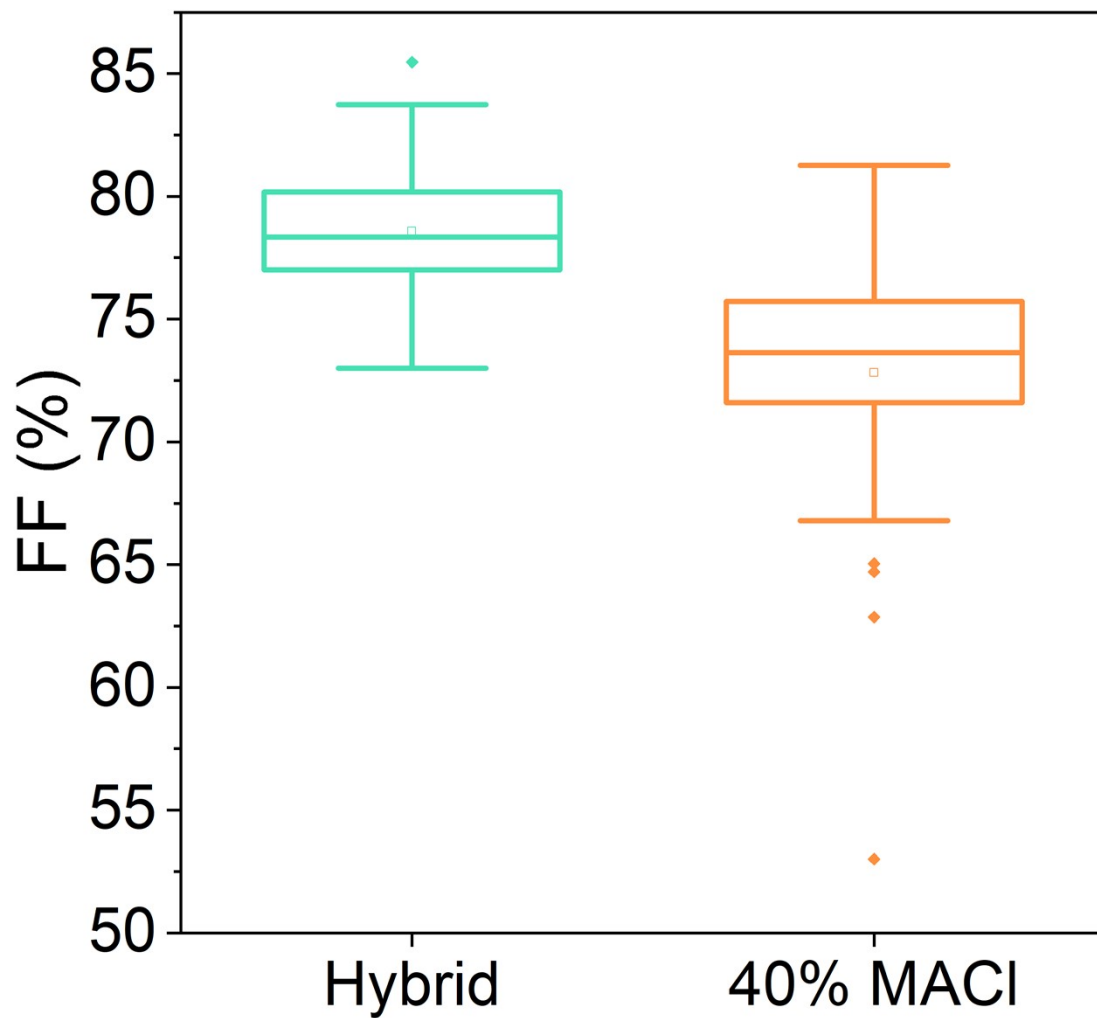


Figure S4: Distribution of fill factor in Hybrid and 40% MACI groups

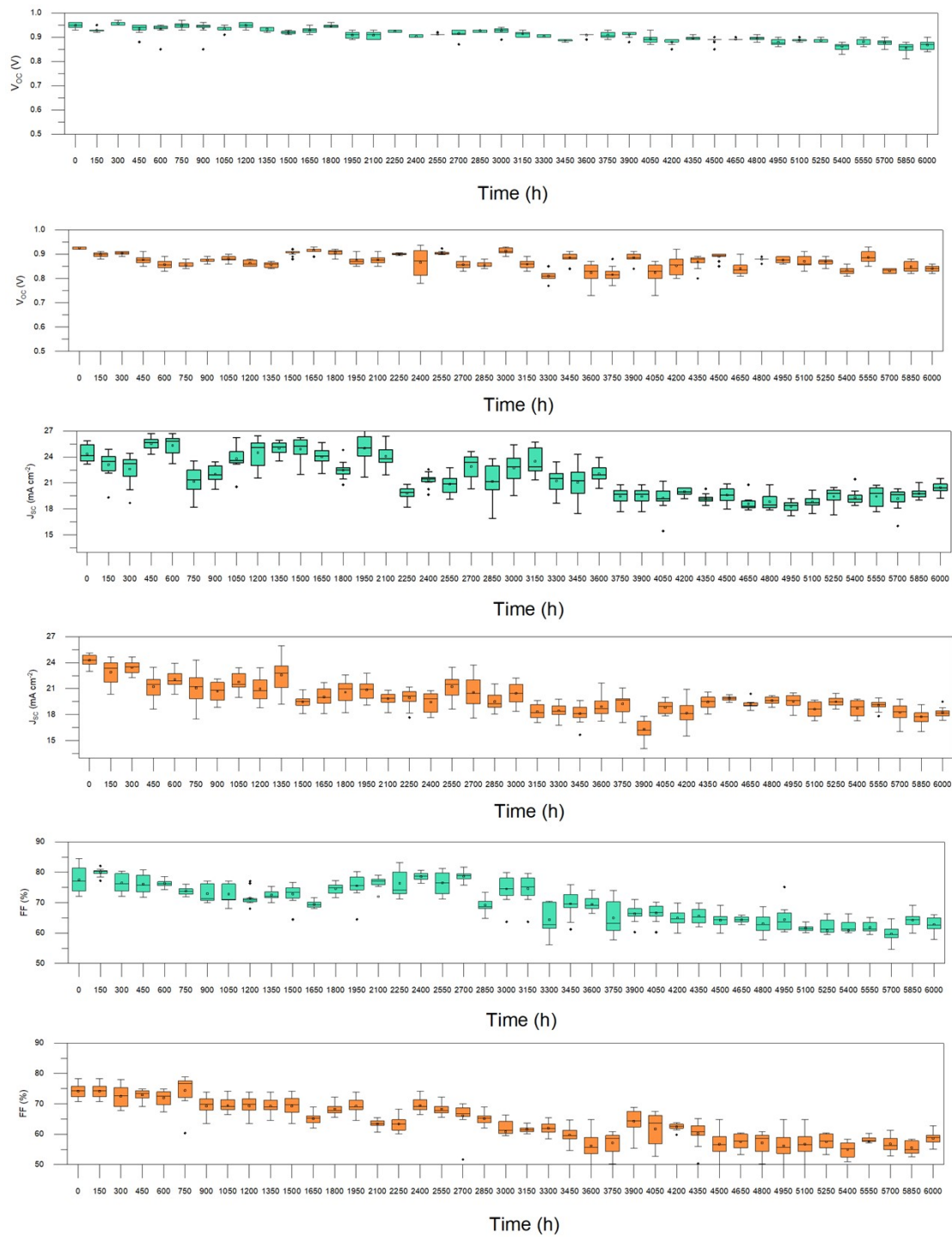


Figure S5:  $V_{oc}$ ,  $J_{sc}$ , FF for 40% MACl group (orange) and Hybrid group (cyan) during 6000h

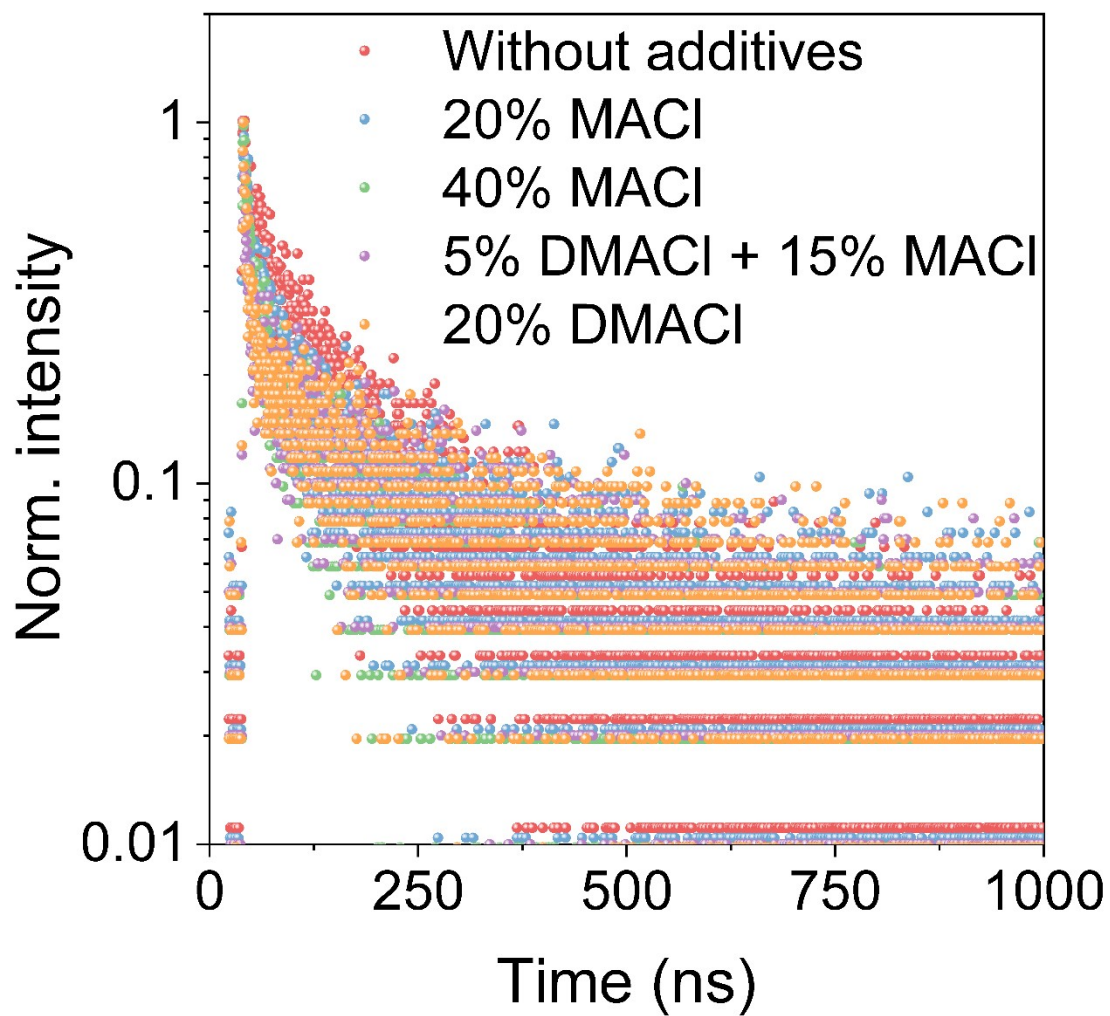


Fig S6: Time-resolved photoluminescence spectra of five perovskite precursors on  $\text{TiO}_2$  substrates



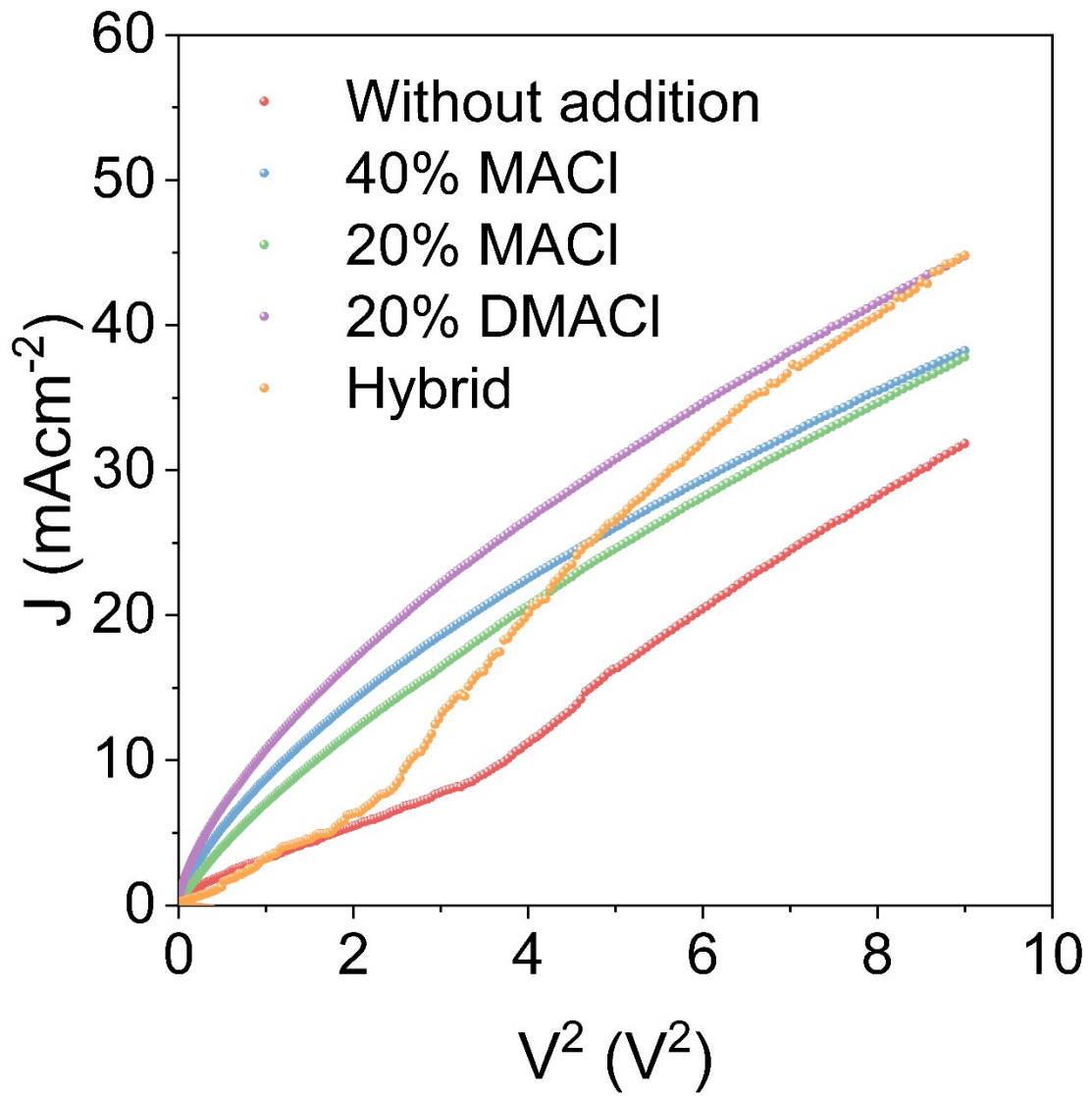


Figure S7: J-V<sup>2</sup> curves of different perovskite films