Supplementary Information

Bromine-Functionalized Carbazole Derivatives in Perovskite Precursors: Defect Passivation for Enhanced Perovskite Photovoltaics

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1. Materials

Cesium iodide (CsI), lead iodide (PbI2), and bathocuproine (BCP) were purchased from Xi'an Yuri Solar Co. Ltd. Formamidinium iodide (FAI) and methylammonium bromide (MABr) were purchased from Greatcell Solar. [2-(3,6-dimethoxy-9H-carbazol-9yl)ethyl] phosphonic acid (MeO-2PACz) , 2-(9H-carbazol-9-yl)ethylphosphonic acid (2PACz) and 2-(3,6-dibromo-9H-carbazol-9-yl)ethylphosphonic acid (Br-2PACz) was purchased from TCI. N, N-Dimethylformamide (DMF), dimethyl sulfoxide (DMSO), isopropanol (IPA), and chlorobenzene (CB) were purchased from Sigma-Aldrich. Ethanol (EtOH) and ethyl acetate (EA) were purchased from Aladdin. [6, 6]-phenyl-C61 butyric acid methyl ester (PCBM, 99%) was purchased from Advanced Election Technology in China. Sodium hydroxide (NaOH, 96%) was purchased from General Reagent. Nickel nitrate hexahydrate ($Ni(NO_3)_2 \cdot 6H_2O$, AR) was purchased from Sinopharm Chemical Reagent Co., Ltd. All materials and solvents were used as received without further purification.

2. Supplementary figures

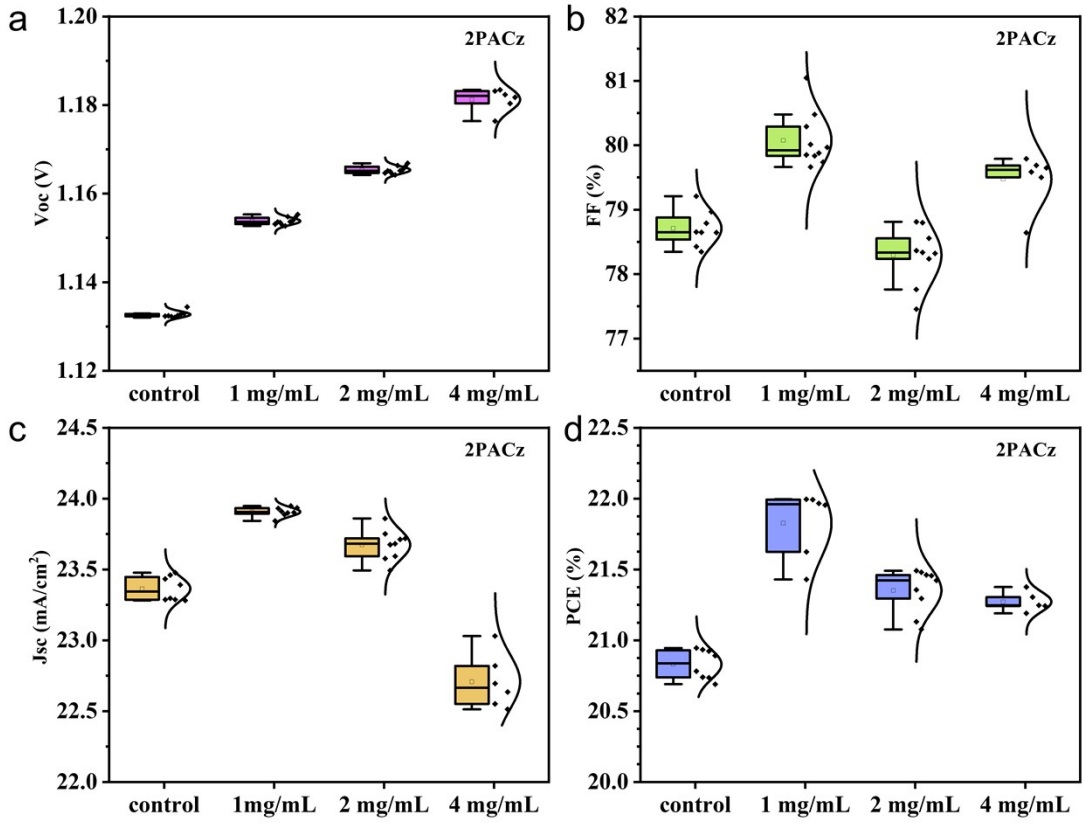

Fig. S1 Photovoltaic parameters of devices with 2PACz doping: (a) open-circuit voltage (*V*oc), (b) fill factor (FF), (c) short-circuit current density (*J*sc), and (d) power conversion efficiency (PCE).

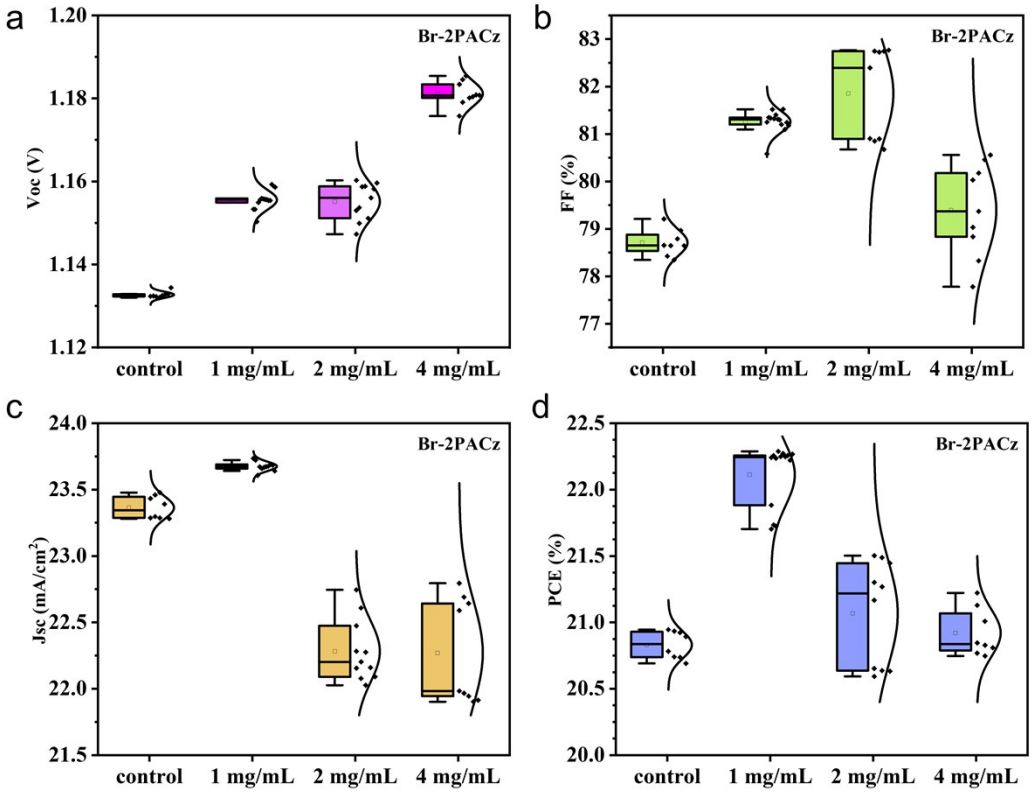

Fig. S2 Photovoltaic parameters of devices with Br-2PACz doping: (a) *V*oc, (b) FF, (c) *J*sc and (d) PCE.

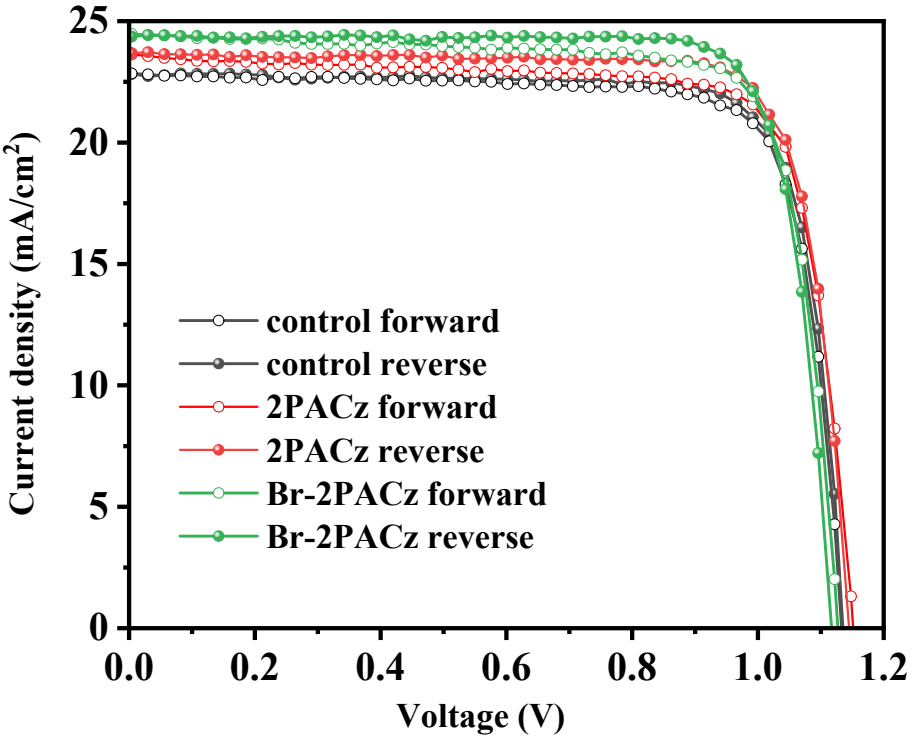

Fig. S3 Forward and reverse *J-V* curves of perovskite solar cells based on the control, 2PACz-incorporated, and Br-2PACz-incorporated devices measured under simulated AM 1.5G illumination (100 mW cm^{-2}).

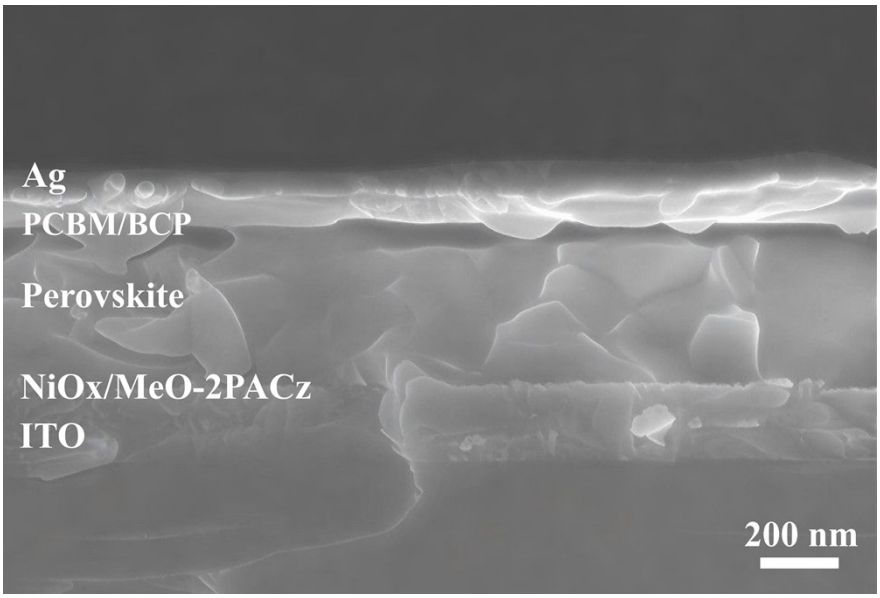

Fig. S4 Cross-sectional SEM image of the complete perovskite solar cell device.

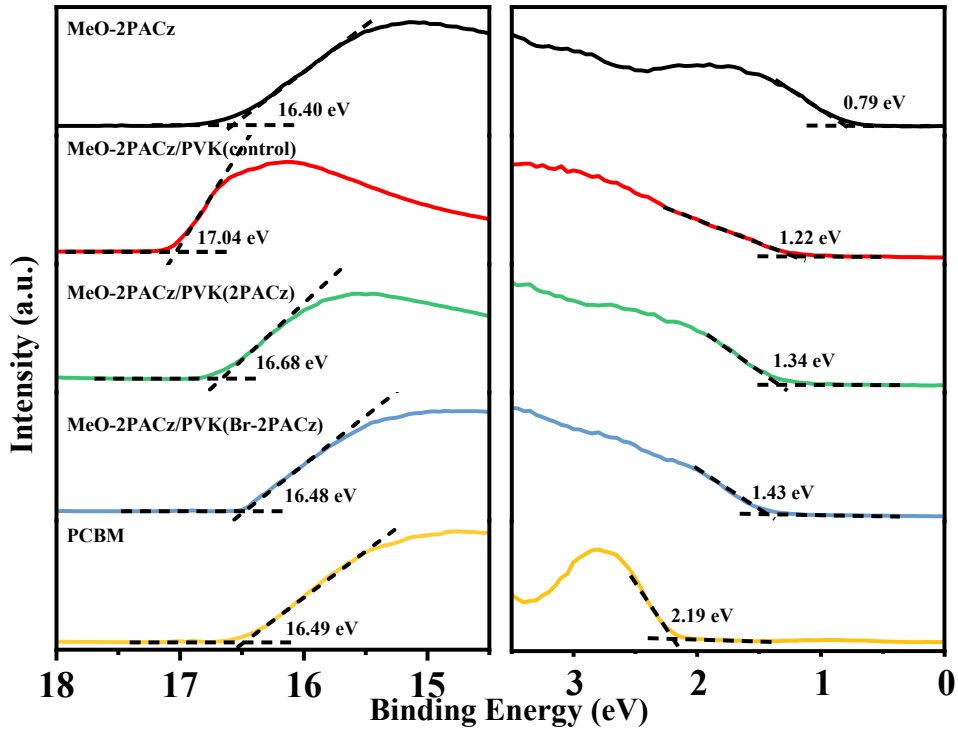

Fig. S5 Ultraviolet photoelectron spectroscopies (UPS) spectra of control perovskite, 2PACz-incorporated, and Br-2PACz-incorporated perovskite (PVK) films.

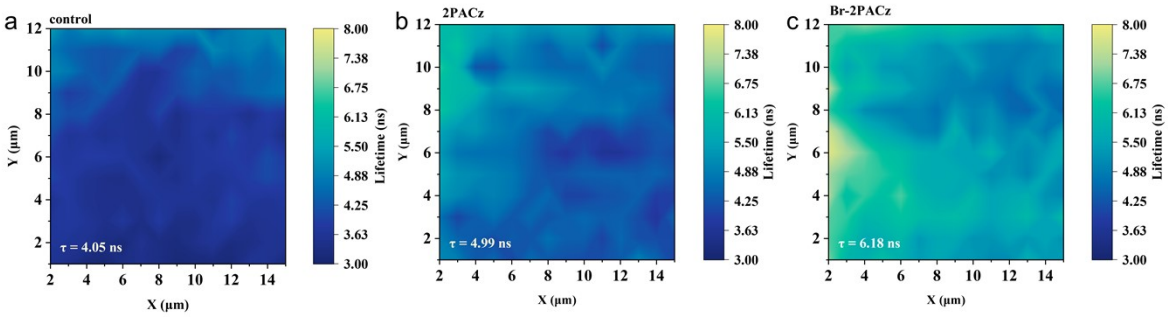

Fig. S6 Time-resolved photoluminescence (TRPL) lifetime maps of perovskite films prepared from the control, 2PACz-incorporated, and Br-2PACz-incorporated precursor solutions.

3. Supplementary tables

Table S1. Atomic percentages derived from XPS survey spectra of control, 2PACz-incorporatedd, and Br-2PACz-incorporated films.

	Cs	Pb	I	C	N	O	Br
control	0.20	1	5.45	3.13	1.77	1.12	0.53
2PACz	0.20	1	4.06	4.94	2.04	1.87	1.23
Br-2PACz	0.12	1	3.12	3.81	1.45	0.89	1.44

Table S2. Summary of secondary electron cutoff (SEC), VBM referenced to E_F, work function (WF) and ionization potential (IP) extracted from the UPS spectra.

	SEC	VBM	WF	IP
MeO-2PACz	16.40	0.79	4.82	5.61
MeO-2PACz/PVK(control)	17.04	1.22	4.18	5.40
MeO-2PACz/PVK(2PACz)	16.68	1.34	4.54	5.88
MeO-2PACz/PVK(Br-2PACz)	16.48	1.43	4.74	6.17
PCBM	16.49	2.19	4.73	6.92