Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Supporting information

Tailoring the molecular size of alkylamine modifiers for fabricating efficient and stable inverted $CsPbI_3$ perovskite solar cells

Zhongyu Liu,[a,b] Hongwei Wang,[a] Haijun Han,[b] Hong Jiang,[b] Ning Liu,[b] Jianwei Wang,[b] Jing Zhang,[b] Tian Cui,*[a] and Xiaohui Liu,*[a,b]

[a] Institute of High Pressure Physics, School of Physical Science and Technology, Ningbo University, Ningbo 315211, China

[b] Department of Microelectronic Science and Engineering, School of Physical Science and Technology, Ningbo University, Ningbo 315211, China

* E-mail: liuxiaohui@nbu.edu.cn; cuitian@nbu.edu.cn.

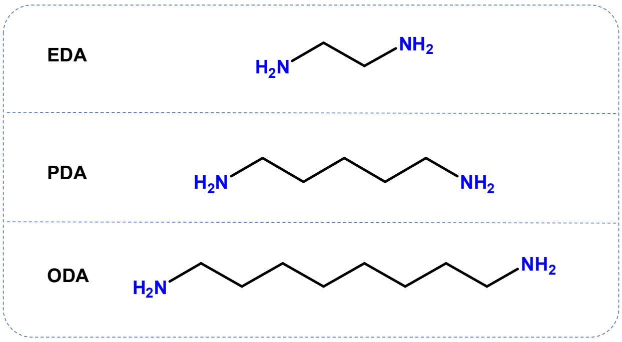

Figure S1. The chemical structures of the three alkylamines (EDA, PDA, and ODA).

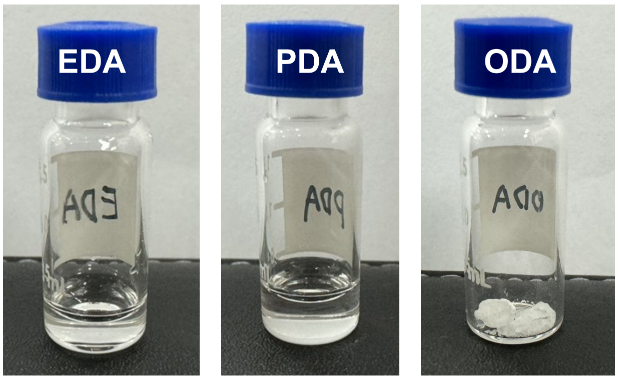

Figure S2. The physical appearances of EDA, PDA, and ODA molecules under normal temperature and pressure.

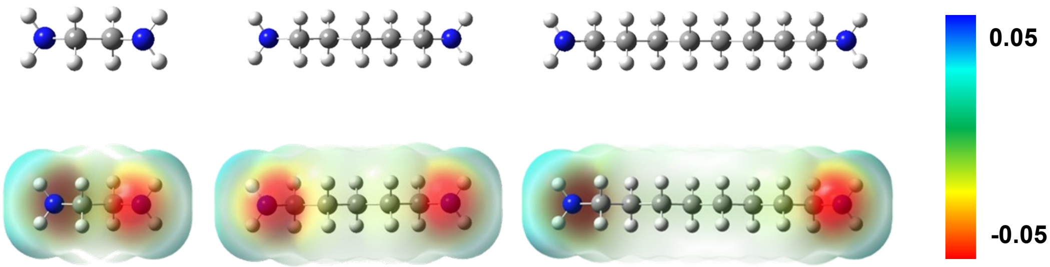

Figure S3. The ESP analysis of EDA, PDA and ODA molecules.

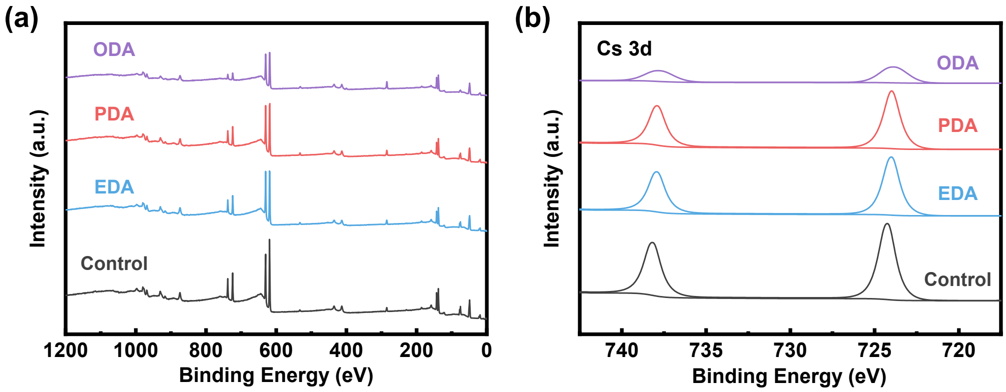

Figure S4. (a) Full-scan XPS spectra of control, EDA, PDA, and ODA treated $CsPbI_3$ films. (b) XPS spectra of Cs 3d.

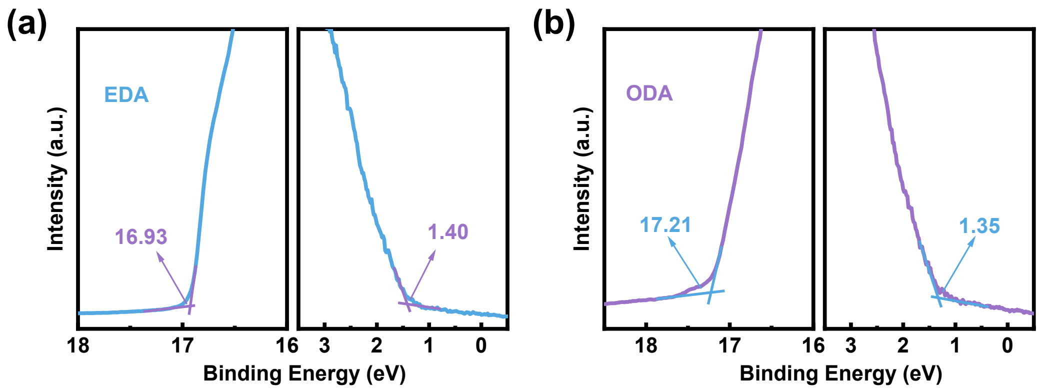

Figure S5. UPS spectra of (a) EDA and (b) ODA treated perovskite films.

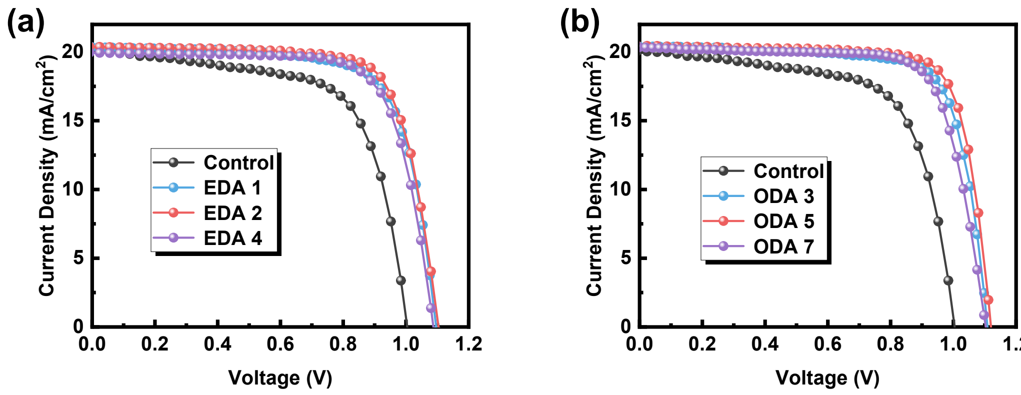

Figure S6. *J-V* curve of devices treated with different concentration of (a) EDA, and (b) ODA.

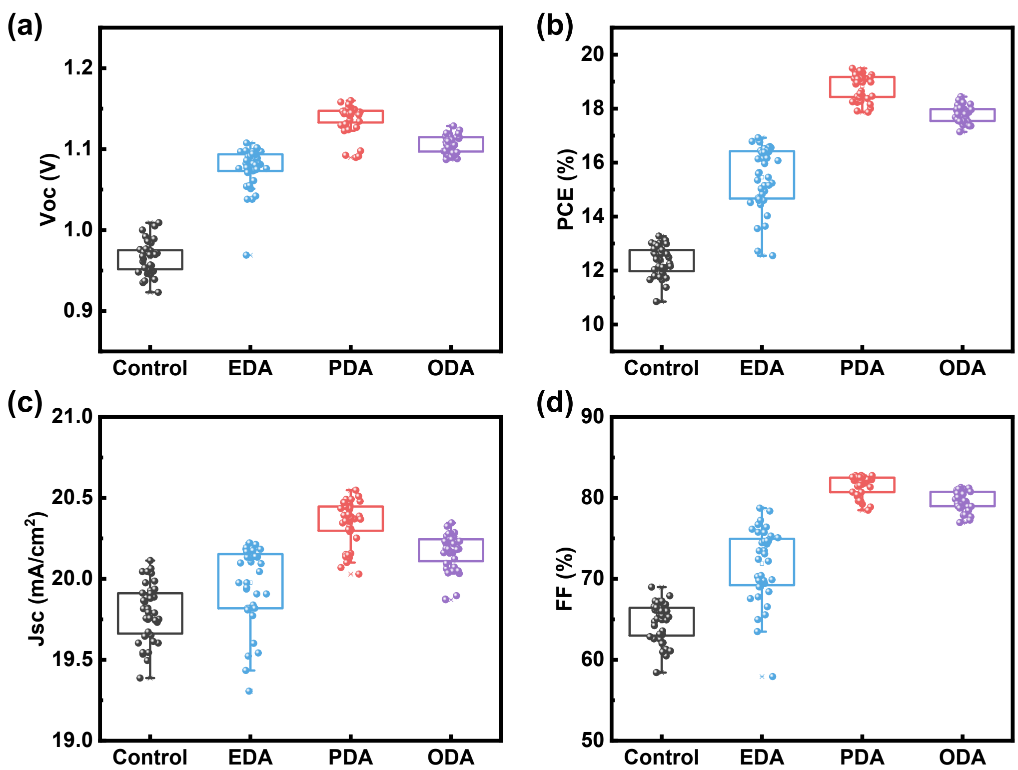

Figure S7. Box data statistics charts of (a) V_{OC}, (b) PCE, (c) J_{SC}, and (d) FF.

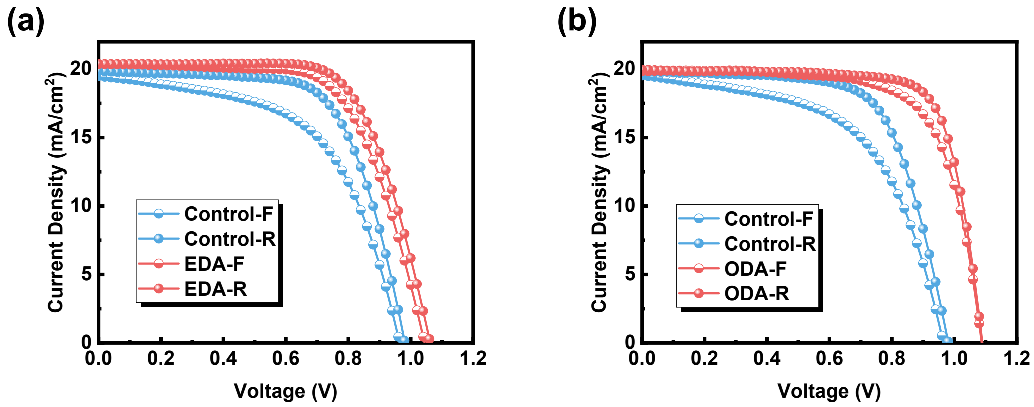

Figure S8. *J*–*V* curves measured in forward and reverse scan directions of (a) EDA, and (b) ODA treated devices.

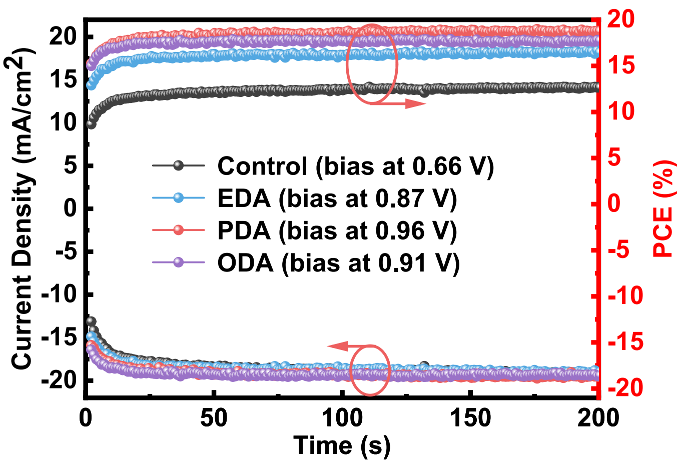

Figure S9. Steady-state photocurrent and output PCE at the maximum power point of control, EDA, PDA, and ODA treated $CsPbI_3$ devices.

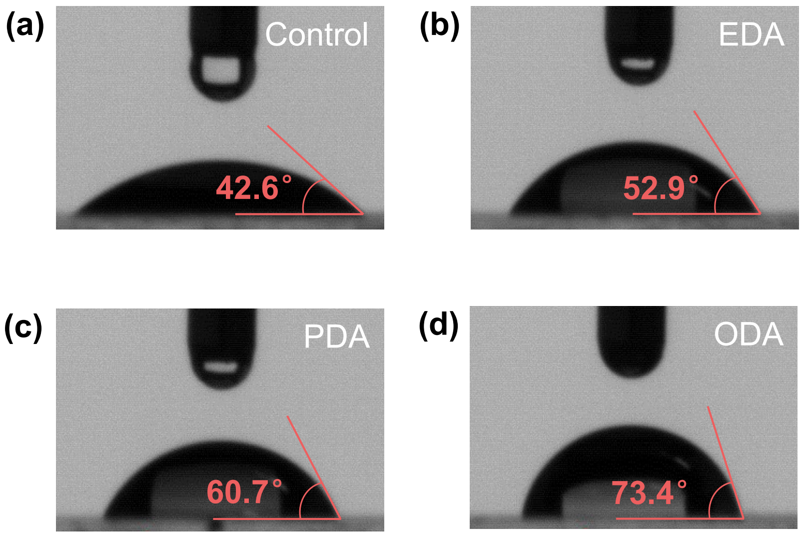

Figure S10. The contact angle of water droplets on (a) control, (b) EDA, (c) PDA, and (d) ODA treated $CsPbI_3$ films, respectively.

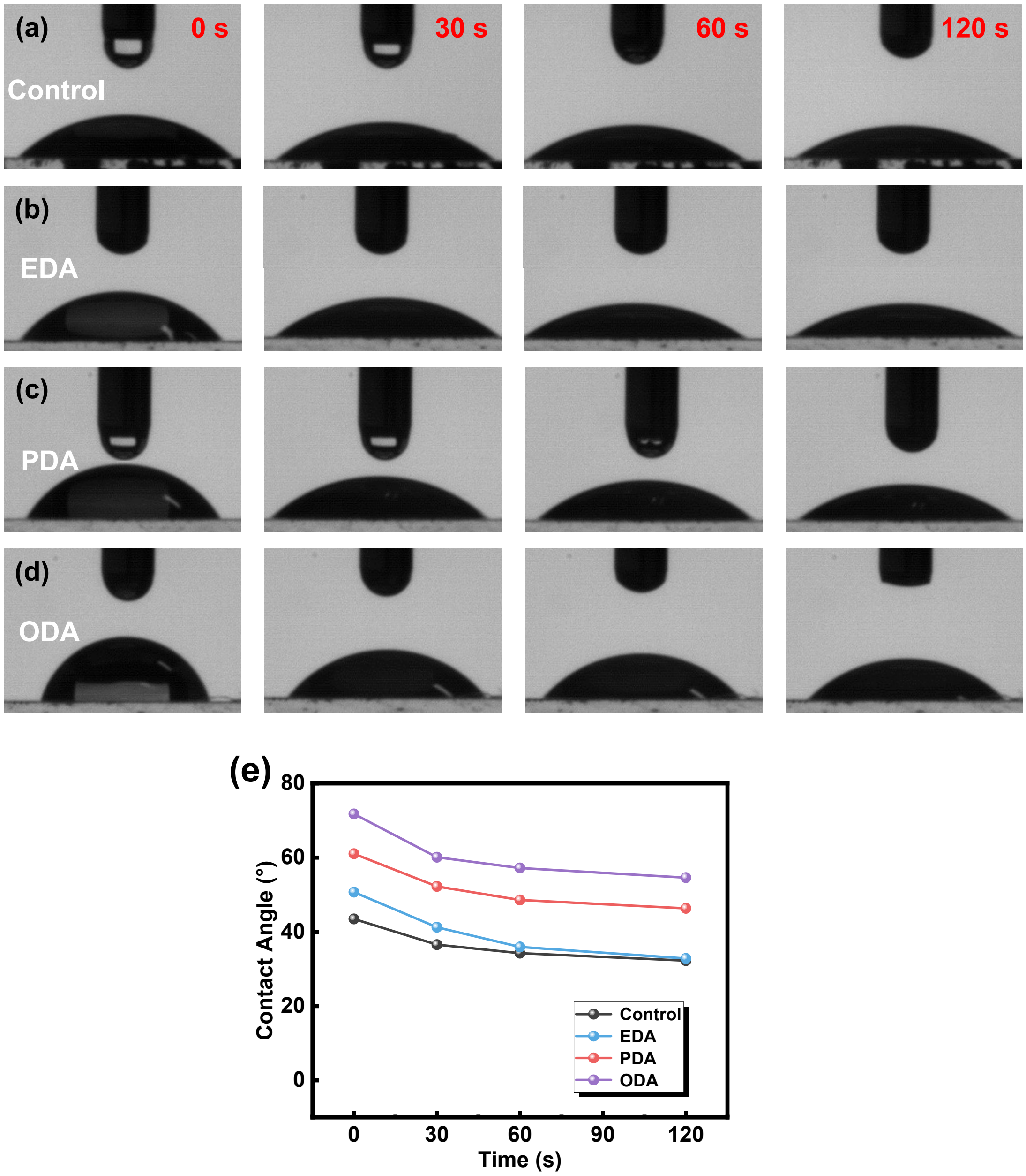

Figure S11. Contact angle images of (a) control, (b) EDA, (c) PDA and (d) ODA treated films captured at different time, respectively; (e) Contact angle versus duration of exposure of four films.

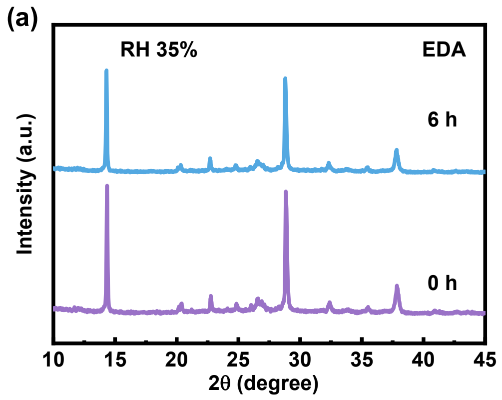

Figure S12. The evolution of XRD patterns of (a) EDA, and (b) ODA treated $CsPbI_3$ films.

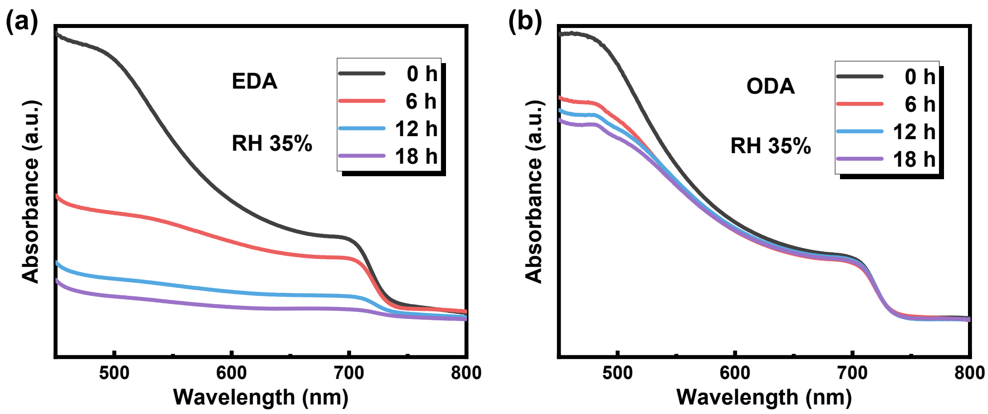

Figure S13. UV-vis spectra of of (a) EDA, and (b) ODA treated $CsPbI_3$ films.

Table S1. The basic physical properties of EDA, PDA, and ODA molecules.

Modifier	EDA	PDA	ODA
Formula	$C_2H_8N_2$	$C_5H_{14}N_2$	$C_8H_{20}N_2$
Physical appearance (25°C)	Liquid	Liquid	Solid
Molecular weight	60.1	102.2	144.2
Melting point (°C)	8.5	9	50
Boiling point (°C)	116	178	225
Vapor pressure (kPa)	1.21	0.13	<0.01

Table S2. Fitting parameters of the TRPL spectra of control, EDA, PDA, and ODA treated $CsPbI_3$ films.

Samples	A_1	τ_1/ns	A_2	τ_2/ns	τ_{avg}/ns
Control	2.32	11.79	88.23	5.37	5.72
EDA	2.16	10.01	1.79	24.71	19.88
PDA	1.06	19.05	1.06	52.26	43.39
ODA	11.23	6.64	0.90	45.22	20.26

Table S3. The band structure parameters of control, EDA, PDA, and ODA treated $CsPbI_3$ films, respectively.

Samples	E_{cutoff} (eV)	E_{onset} (eV)	VB (eV)	CB (eV)	E_F (eV)
Control	16.84	1.30	5.68	4.00	4.38
EDA	16.93	1.40	5.69	4.01	4.29
PDA	16.99	1.56	5.79	4.11	4.23
ODA	17.21	1.35	5.36	3.68	4.01

Table S4. The photovoltaic parameters of devices based on different concentrations of EDA, PDA, and ODA solutions treatment.

Sample (mg/mL)	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)
Control	0.997	20.04	67.24	13.43
EDA 1	1.096	20.24	73.32	16.26
EDA 2	1.105	20.18	75.28	16.79
EDA 4	1.077	20.12	72.41	15.69
PDA 4	1.117	20.35	82.95	18.85
PDA 6	1.151	20.39	83.18	19.52
PDA 8	1.105	20.27	82.31	18.43
ODA 3	1.108	20.24	80.45	18.04
ODA 5	1.116	20.26	81.34	18.39
ODA 7	1.101	20.21	77.38	17.22

Table S5. The photovoltaic parameters of the control, EDA, PDA, and ODA treated $CsPbI_3$ PSCs.

Sample	V_{OC} (V)	J_{SC} (mA/cm^2)	FF (%)	PCE (%)
Control	0.997 (0.966±0.0194)	20.04 (19.79±0.18)	67.24 (64.77±2.59)	13.43 (12.37±0.55)
EDA	1.105 (1.077±0.025)	20.18 (19.98±0.24)	75.28 (71.87±4.43)	16.79 (15.46±1.14)
PDA	1.151 (1.137±0.017)	20.39 (20.34±0.13)	83.18 (81.57±1.24)	19.52 (18.86±0.46)
ODA	1.116 (1.106±0.010)	20.26 (20.17±0.11)	81.34 (79.67±1.18)	18.39 (17.78±0.30)