

ARTICLE

Supporting information

Asymmetric Alkyl Diamine Based Dion-Jacobson Low-Dimensional Perovskite Solar Cells with Efficiency Exceeding 15%

Weidong Zhao,^a Qingshun Dong,^{*a} Jiangwei Zhang,^{*b} Shi Wang,^a Min Chen,^c Chunyi Zhao,^d Mingyu Hu,^c Shengye Jin,^d Nitin P. Padture,^c and Yantao Shi^{*a}

^aState Key Laboratory of Fine Chemicals, Department of Chemistry, School of Chemical Engineering, Dalian University of Technology, Dalian, 116024, China. Email: dongqs@dlut.edu.cn; shiyantao@dut.edu.cn

^bState Key Laboratory of Catalysis, Dalian Institute of Chemical Physics, Chinese Academy Sciences Dalian, 116023, China. Email: jwzhang@dicp.ac.cn

^cSchool of Engineering, Brown University, Providence, Rhode Island 02912, United States.

^dState Key Laboratory of Molecular Reaction Dynamics, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian, 116023, China.

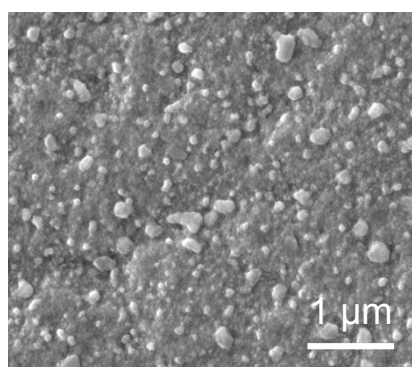


Fig. S1. Top-view SEM images of the (DMAPA)PbI₄ perovskite film.

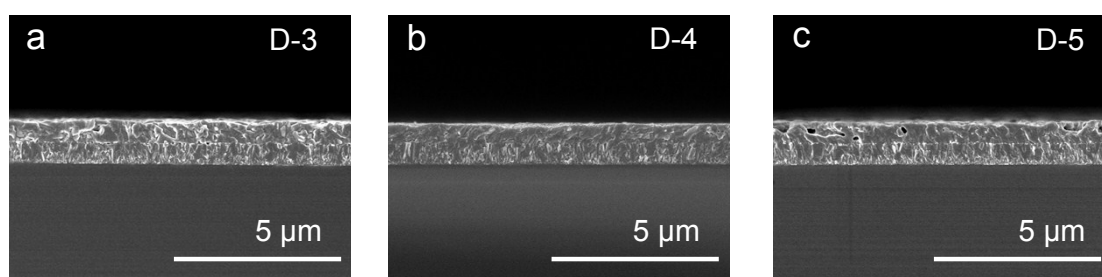


Fig. S2. Wide range cross-sectional SEM images of the D-3 (a), D-4 (b) and D-5 (c) perovskite films, respectively.

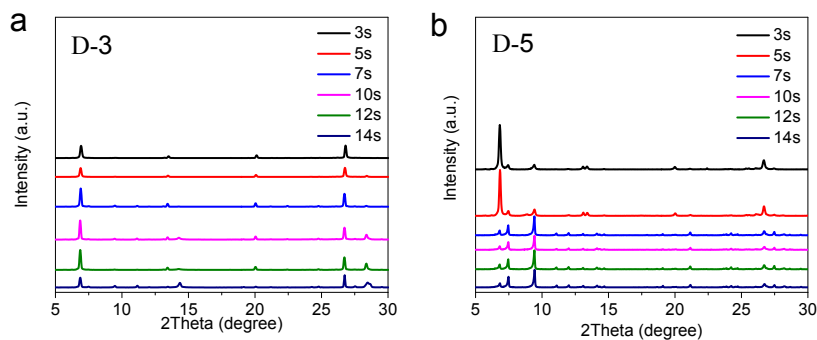


Fig. S3. XRD pattern of D-3 (a) and D-5 (b) films at the deposition time of 3s, 5s, 7s, 10s, 12s, 14s, respectively.

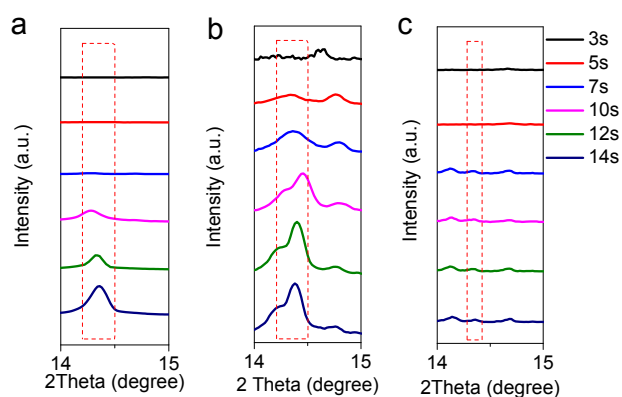


Fig. S4. Detail XRD peak evolution at 14.4° for the D-3 (a), D-4 (b) and D-5 (c) perovskite films, respectively.

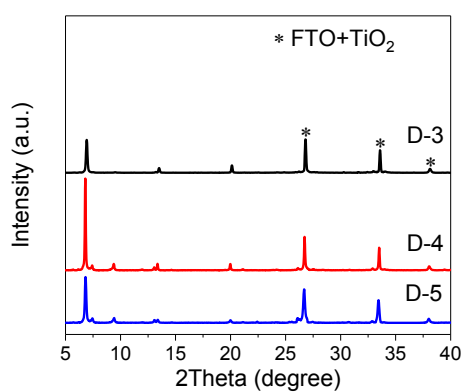


Fig. S5. XRD patterns for the D-3, D-4, and D-5 films collected at 3 s after the start of hot casting.

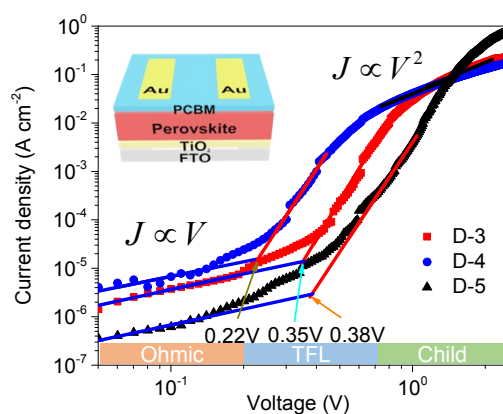


Fig. S6. Space-charge limited current of the electron only devices for the D-3, D-4, and D-5 perovskite films. Insert: device structure of the electron only device.

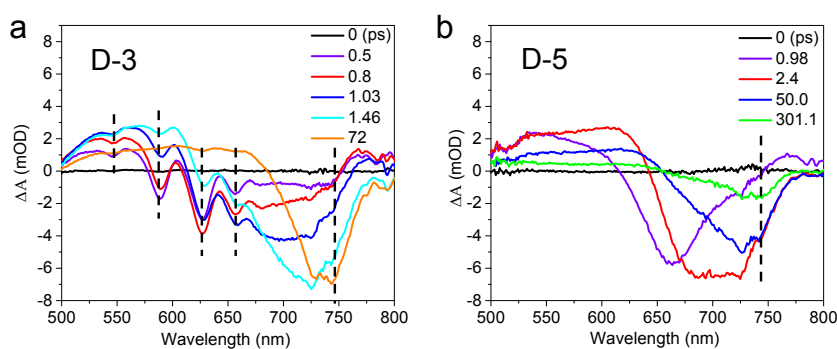


Fig. S7. Transient absorption (TA) spectra with various delay times for D-3 (a) and D-5 (b) perovskite films, respectively.

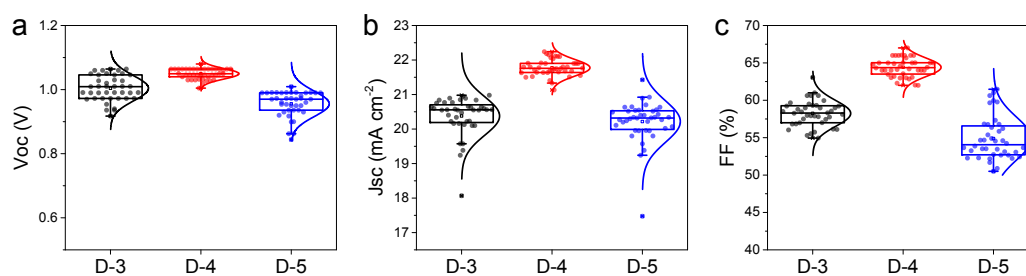


Fig. S8. Statistics of the V_{oc} (a), J_{sc} (b) and FF (c) from the photovoltaic parameters of the devices based on D-3, D-4, and D-5 DMAPA LD perovskites, respectively.

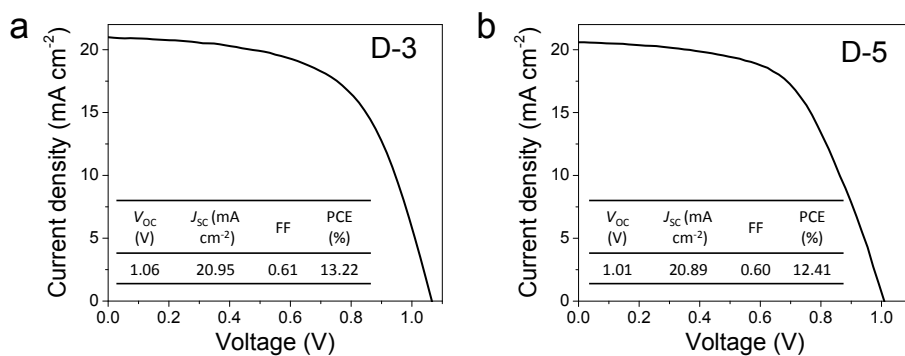


Fig. S9. Champion J - V curves for the D-3 (a) and D-5 (b) perovskite devices.

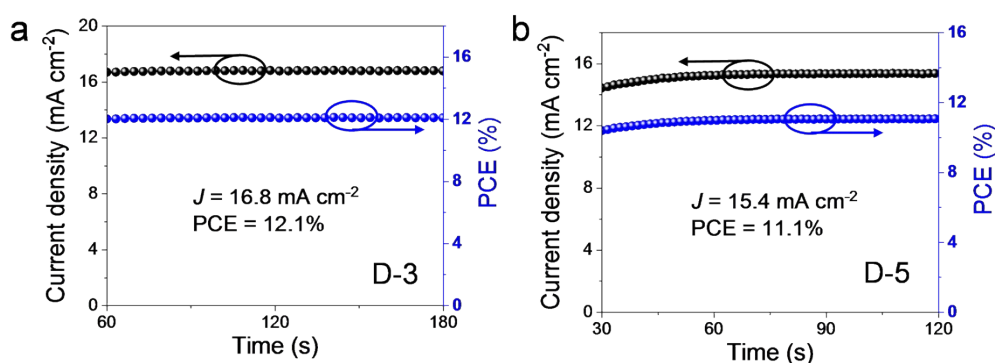


Fig. S10. Stabilized power outputs and current densities at maximum power point for the D-3 (a) and D-5 (b) LD perovskite solar cells.

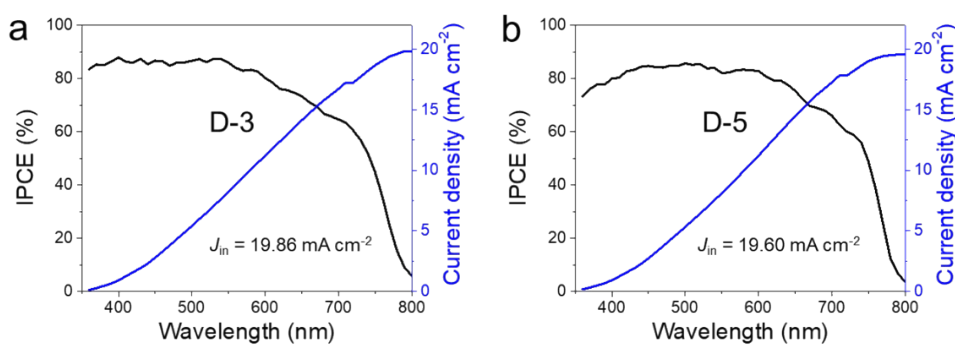


Fig. S11. IPCE spectrum and integrated short circuit current density as a function of wavelength for the D-3 and D-5 LD PSCs, respectively.

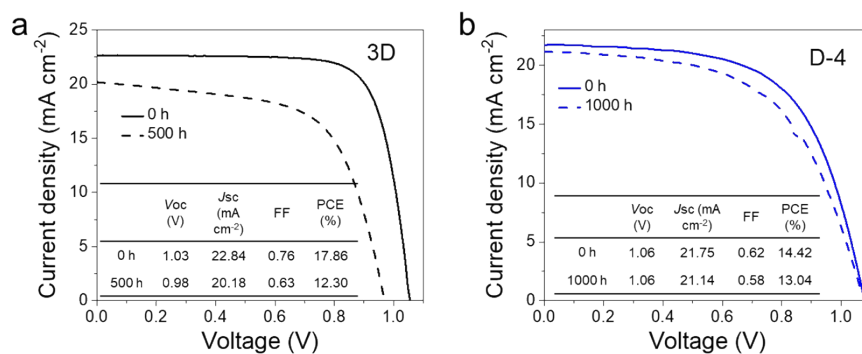


Fig. S12. The J - V curves and related photovoltaic parameters of the devices based on 3D (a) and D-4 (b) perovskite before and after thermal aging in air.

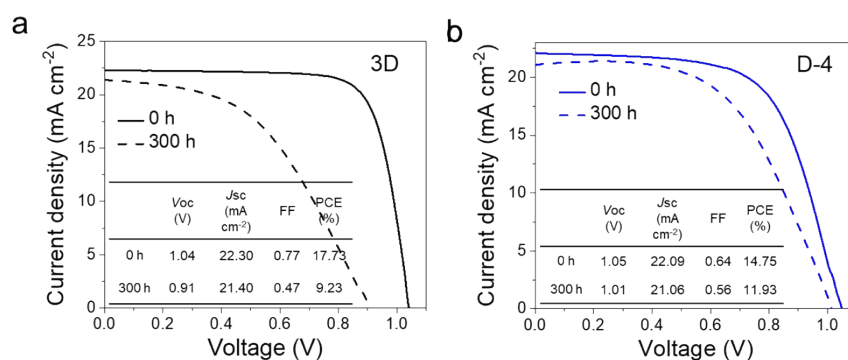


Fig. S13. The J - V curves and related photovoltaic parameters of the devices based on 3D (a) and D-4 (b) perovskite before and after the 300-hour 1 sun illumination in air.

Table S1. Crystal Data and Structure Refinement for (DMAPA)PbI₄.

Empirical formula	C ₅ H ₁₆ I ₄ N ₂ Pb
Crystal system	orthorhombic
Space group	Pbca
a/Å	18.435(2)
b/Å	8.6432(12)
c/Å	20.797(4)
α/°	90
β/°	90
γ/°	90
Volume(Å ³)	3313.7(9)
Z	8
Density (g cm ⁻³)	3.283
Reflections collected	3988
Independent reflections	3815 [Rint = 0.0235, Rsigma = 0.0438]
Data/restraints/parameters	3815/45/113
Final R indexes [I>=2σ (I)]	R1 = 0.0311, wR2 = 0.0648
Final R indexes [all data]	R1 = 0.0475, wR2 = 0.0718
Largest diff. peak/hole / e Å ⁻³	0.75/-0.58

Table S2. Parameters of the TRPL spectroscopy of the D-3, D-4, and D-5 perovskite.

Samples	τ _{ave} (ns)	τ ₁ (ns)	τ ₂ (ns)	A ₁	A ₂
D-3	18.4	6.38	23.9	0.634	0.37
D-4	34.5	8	40.9	0.54	0.436
D-5	5.6	0.824	7.48	0.81	0.235

Table S3. The average and champion photovoltaic parameters of solar cells based on D-3, D-4, and D-5 DMAPA LD perovskites.

Samples		V_{oc} (V)	J_{sc} (mA cm ⁻²)	FF	PCE (%)
D-3	Average	1.0 ± 0.04	20.38 ± 0.55	0.58 ± 0.017	11.91 ± 0.68
	Champion	1.06	20.95	0.61	13.22
D-4	Average	1.04 ± 0.02	21.90 ± 0.21	0.64 ± 0.011	14.71 ± 0.33
	Champion	1.08	22.04	0.65	15.16
D-5	Average	0.96 ± 0.04	20.22 ± 0.60	0.55 ± 0.038	10.6 ± 0.68
	Champion	1.01	20.89	0.60	12.41