

Incorporating Self-assembled Silane-crosslinked Carbon Dots into Perovskite Solar Cells to Improve Efficiency and Stability

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Keywords: Self-assembly, CDs-SAM, Moisture stability, tunneling layer, Perovskite solar cells.

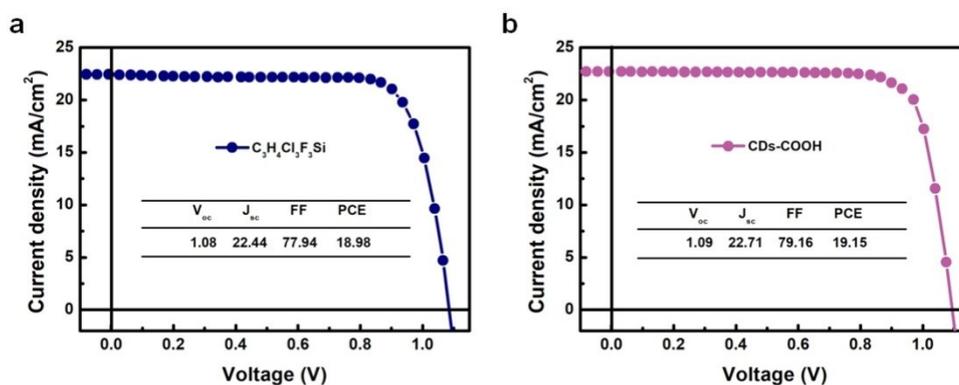


Figure S1a) $J-V$ curves of PSCs with $C_3H_4Cl_3F_3Si$ layer; **b)** $J-V$ curves of PSCs with CDs-COOH layer.

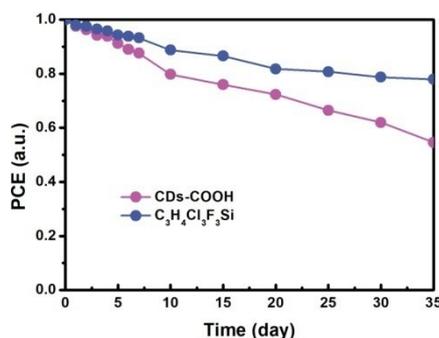


Figure S2 Photovoltaic performance as a function of storage time for the CDs-COOH and $C_3H_4Cl_3F_3Si$ based devices in ambient environment without encapsulation,

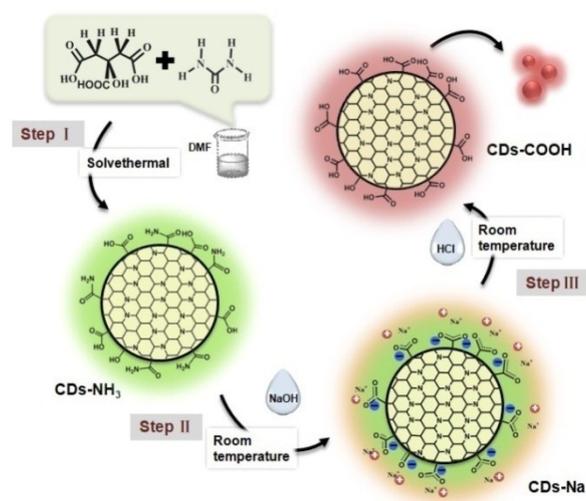


Figure S3 A possible growth mechanism for CDs-COOH.

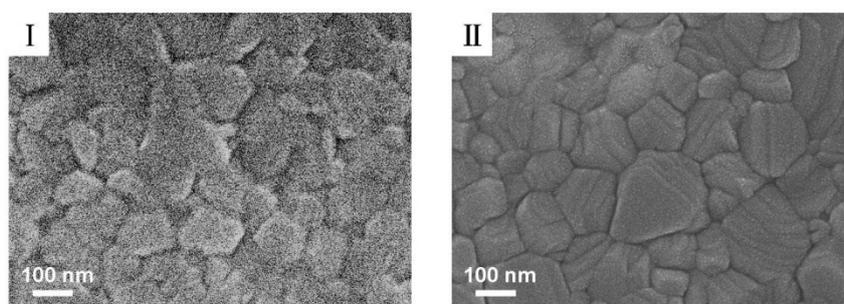


Figure S4 Cross-section SEM images of PSCs with CDs-COOH and C₃H₄Cl₃F₃Si.

Table S1 The performances of all devices, including R_s , V_{oc} , J_{sc} , FF, best PCE, and average PCE.

Devices	R_s (ohm)	V_{oc} (V)	J_{sc} (mA/cm ²)	FF (%)	PCE (best, %)	PCE (average, %)
normal	104.73	1.08	21.37	76.14	17.65	17.21
Si	97.19	1.08	22.44	77.94	18.98	18.51
CDs-SAM	65.47	1.10	23.21	82.56	21.12	20.59
CDs-COOH	68.51	1.09	22.71	79.16	19.68	19.15

Experimental Section

CDs-COOH synthesis

1 g citric acid and 2 g urea were added into 10 mL DMF and reacted at 160 °C for 6 h under solvothermal condition. The obtained solution was mixed with 20 mL NaOH aqueous solution (50 mg mL⁻¹) and centrifuged at 15000 r min⁻¹ for 10 min. The collected precipitate was further dissolved in 10 mL water and centrifuged at 15 000 r min⁻¹ for 10 min. 100 mg freeze-dried precipitate was added

into 20 mL HCl solution (5 wt%) and centrifuged at 15000 r min⁻¹ for 10 min. The collected precipitate was further dissolved in 10 mL water and stirred for 10 min. The obtained solution were centrifuged at 15 000 r min⁻¹ for 10 min and freeze-dried to produce the brown-red CDs-COOH.

Device fabrication

All the spin coating process was conducted in dehumidified atmosphere (RH<30%) at room temperature (~25°C). The Poly(bis(4-phenyl)(2,4,6-trimethylphenyl)amine) (PTAA) hole transport layers, doped with 1 wt% F4-TCNQ, was first deposited on cleaned ITO substrate by spin coating 5 mg/mL PTAA solution at 4,000 rpm for 30 s and annealed at 100 °C for 15 min. The perovskite precursor solution was prepared via dissolving 462 mg MAI, 159 mg PbI₂, and 78 uL DMSO(molar ratio of 1:1:1) in 600 uL DMF. The solution was stirred overnight at room temperature and filtered with 0.22 μm PVDF filters. Then, the perovskite films were made by spin-coating the perovskite precursor solution onto the prepared PTAA substrates at 4,000 rpm for 30 s and annealed at 100 °C for 2 min. Subsequently, the CDs-COOH solution was spin-coated onto the perovskite films at 5,000 r.p.m. for 30 s. The films were put on a hotplate and covered with a glass petri dish to anneal at 100 °C for another 10 min. 5 ml of trichloro(3,3,3-trifluoropropyl)silane was added at the edge of the petri dish during the thermal annealing process. For control devices, the perovskite precursor solution was spin-coated onto top of the PTAA substrates at 4,000 rpm for 30 s and then annealed at 100 °C for 10 min. C60 (30 nm) and Bphen (6 nm) were then thermally evaporated as the buffer layers. The devices were completed by the evaporation of 100 nm Ag electrode. The device working area was defined by the overlap of ITO and the Ag cathode. Typical dimension of the device area was 2.0 mm × 2.0 mm.

Film and device characterization

The photocurrent-voltage curves were measured using a Keithley 2601 source meter and Oriel 67005, 150W Solar Simulator. The EQE was obtained using a Newport Oriel IPCE measurement kit. The FTIR spectra were collected in the transmittance mode on the IR spectrometer instrument. UV-Vis absorption spectra were recorded using a UV-1700 spectrometer. The X-ray diffraction (XRD) patterns were carried out on a Rigaku Ultima IV diffractometer using Cu Ka radiation. The scanning electron microscopy (SEM) images were taken from a ZEISS Sigma FE-SEM.