

Supporting information

N-type branched shoulder chain small molecule electronic interface layer for inverted perovskite solar cells

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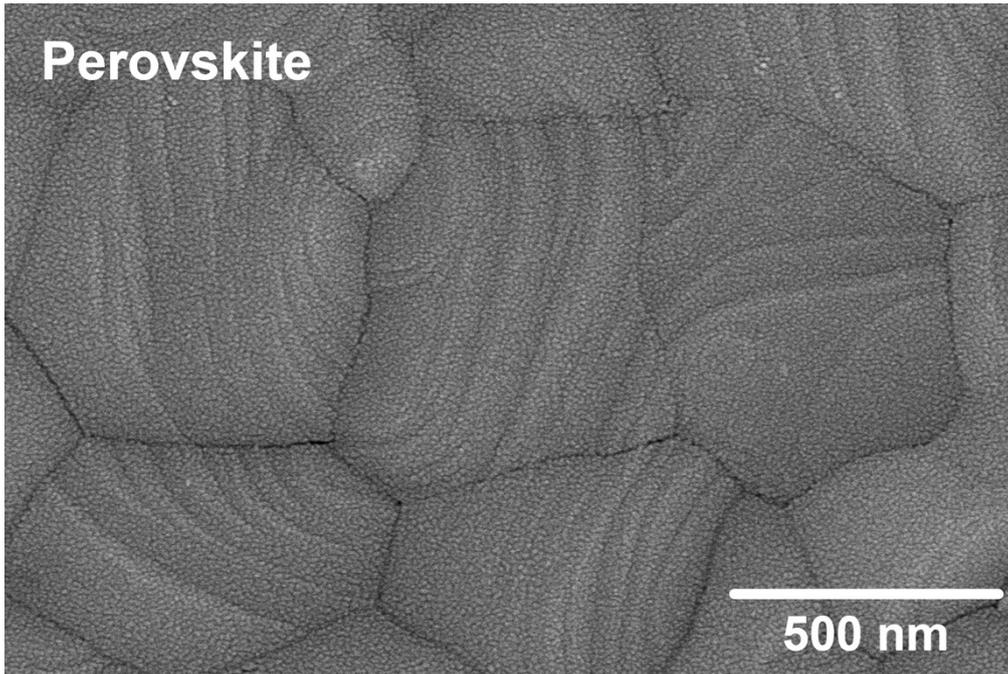


Fig. S1. Surface SEM image of perovskite layer on the PTAA substrate.

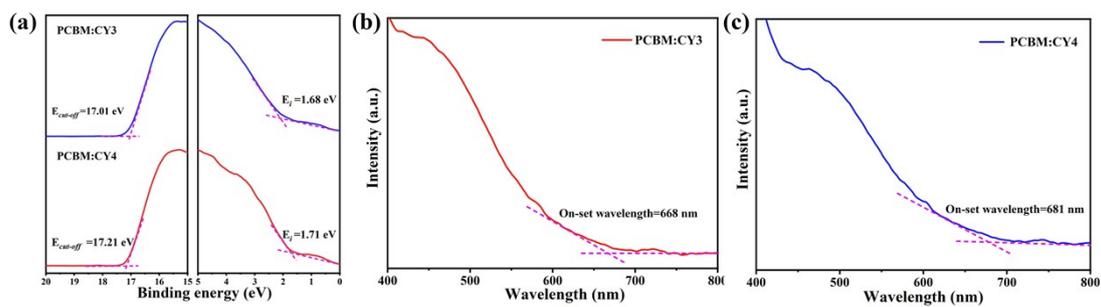


Fig. S2. (a) UPS spectrum of PCBM:CY3 and PCBM:CY4 ETLs, secondary electron cutoff (left) and valence band maximum (right). (b, c) UV-vis of PCBM:CY3 and PCBM:CY4 ETLs.

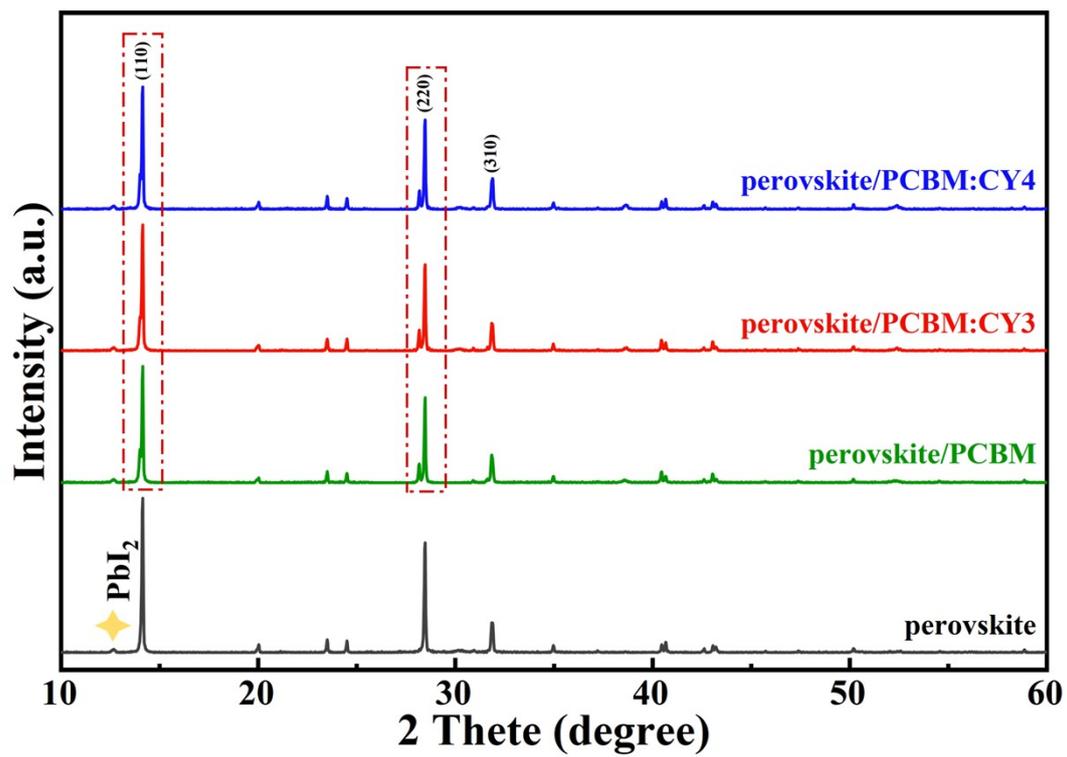


Fig. S3. XRD patterns of perovskite, perovskite/PCBM, perovskite/PCBM:CY3, and perovskite/PCBM:CY4 layers.

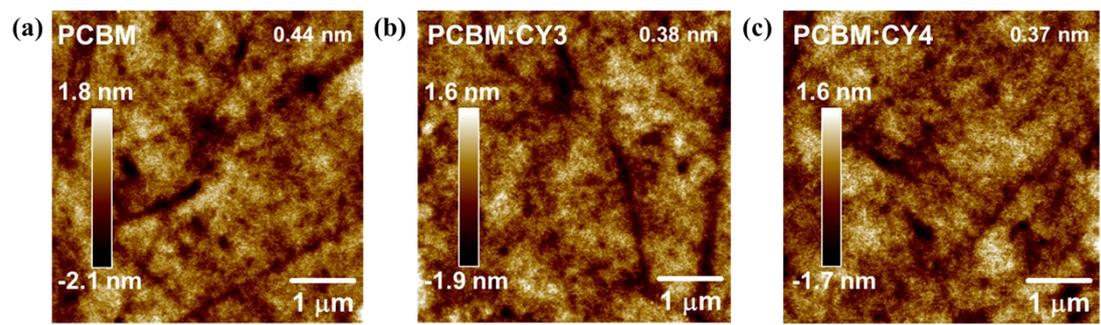


Fig. S4. AFM images of pure (a) PCBM, (b) PCBM:CY3, and (c) PCBM:CY4 deposited on glass substrates.

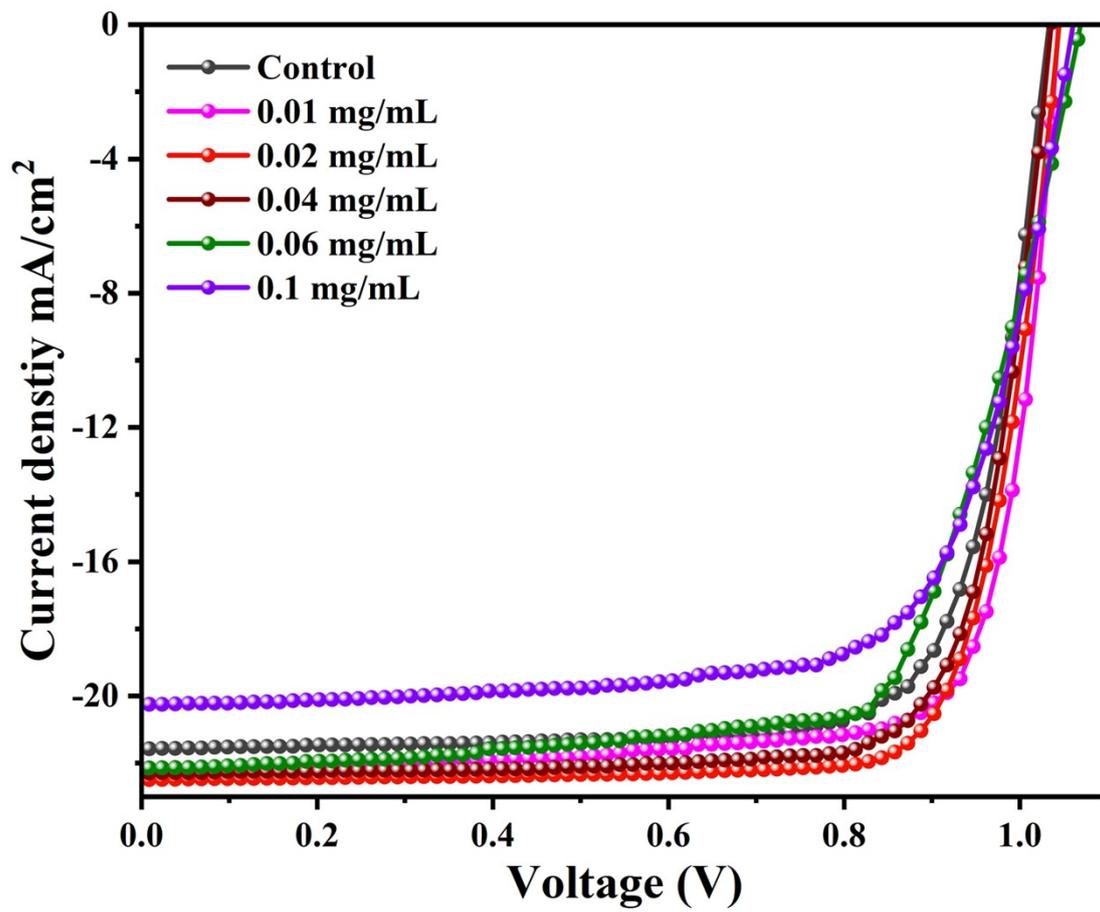


Fig. S5. J - V curves of PSCs prepared based on PCBM:CY3 at different concentrations.

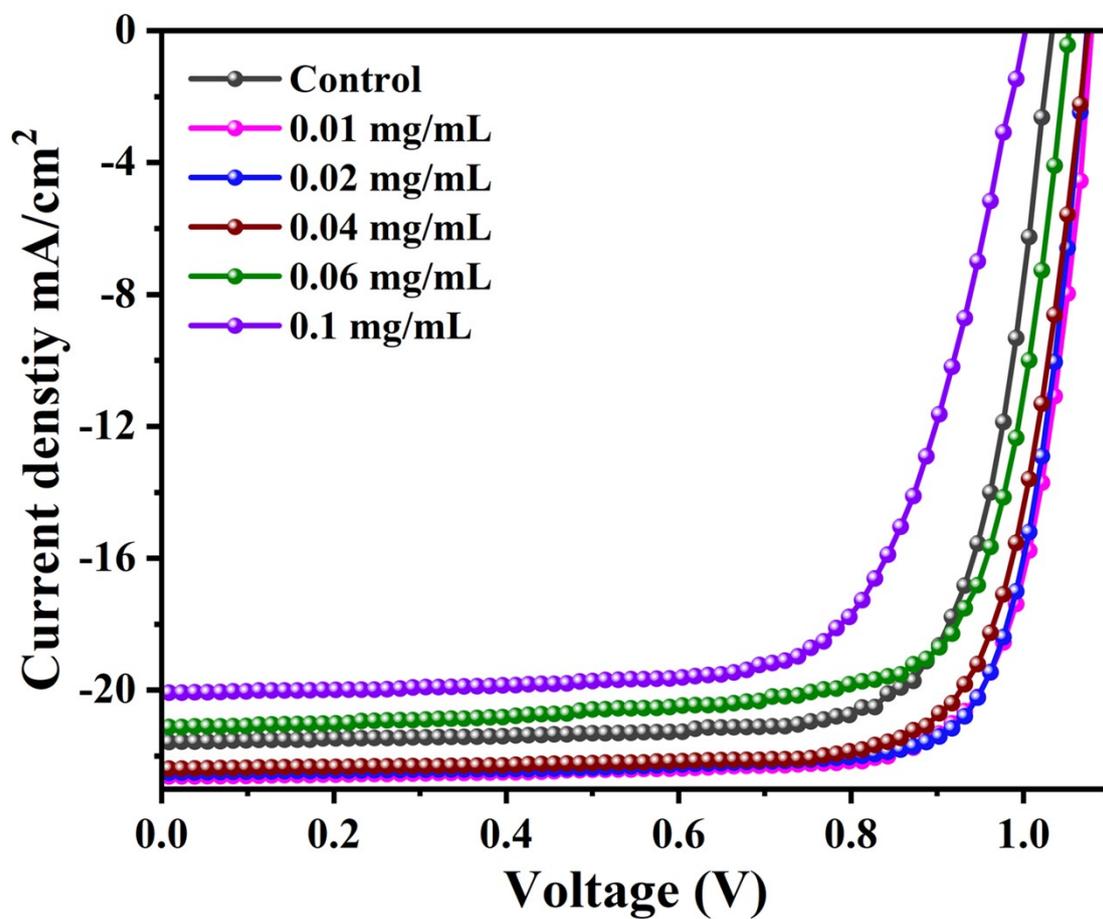


Fig. S6. J - V curves of PSCs prepared based on PCBM:CY4 at different concentrations.

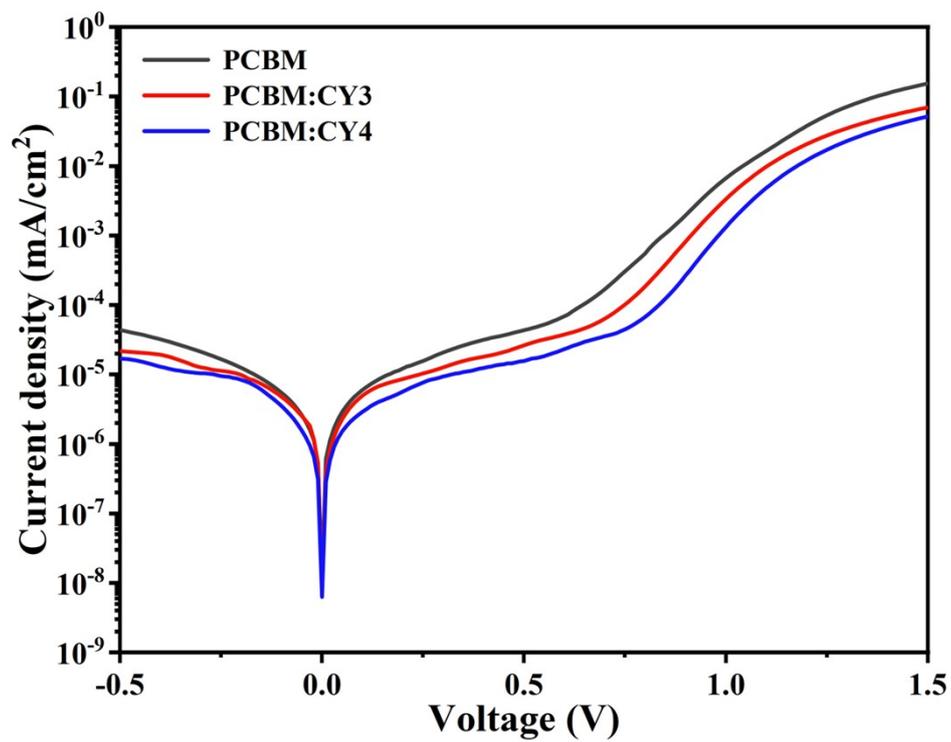


Fig. S7. Dark state J - V curves of PSCs with PCBM, PCBM:CY3, and PCBM:CY4 as ETL.

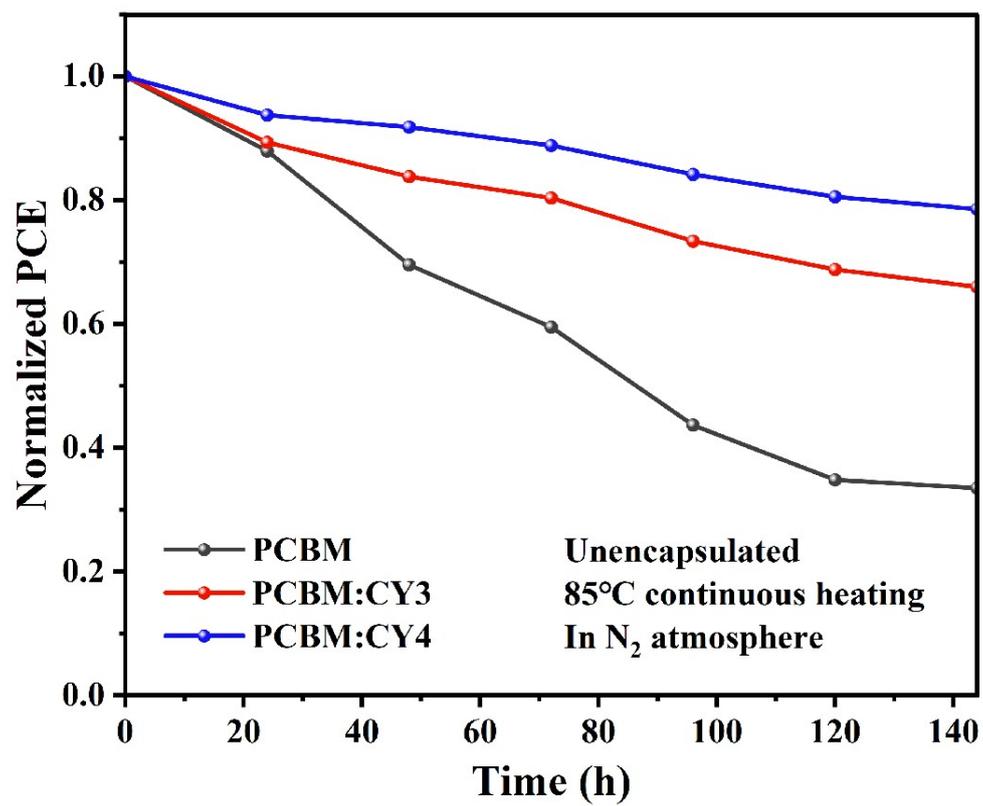


Fig. S8. Thermal stability of unpackaged PSCs devices with PCBM, PCBM:CY3 and PCBM:CY4 as ETL at 85°C in N₂ atmosphere.

Table S1. TRPL parameter fitting results of three different hybrid ETLs covered on perovskite films.

sample	τ_1 (ns)	A_1	τ_2 (ns)	A_2	τ_{avg} (ns)
PCBM	4.22	0.16	43.67	0.06	35.59
PCBM:CY3	2.33	0.63	35.13	0.03	16.04
PCBM:CY4	1.89	1.12	34.46	0.03	12.58

TRPL double exponential decay fitting function and average carrier lifetime calculation

formula

$$I(t) = I_0 + A_1 \exp\left(-\frac{t}{\tau_1}\right) + A_2 \exp\left(-\frac{t}{\tau_2}\right) \quad \text{* MERGEFORMAT}$$

(1)

$$\tau_{\text{ave}} = \frac{(A_1\tau_1^2 + A_2\tau_2^2)}{A_1\tau_1 + A_2\tau_2} \quad \text{* MERGEFORMAT (2)}$$

I_0 is the background constant, A_1 and τ_1 are the fast decay process parameters, and A_2 and τ_2 are the slow decay process parameters.

Table S2. Photovoltaic performance parameter of PSCs prepared based on PCBM:CY3 at different concentrations.

Concentration (mg mL ⁻¹)	J_{SC} (mA cm ⁻²)	V_{OC} (V)	FF (%)	PCE (%)
Control	21.59	1.03	77.06	17.20
0.01	22.20	1.04	78.17	18.01
0.02	22.60	1.05	79.12	18.78
0.04	22.30	1.04	78.29	18.15
0.06	21.20	1.03	77.01	16.82
0.1	19.96	1.00	71.24	14.22

Table S3. Photovoltaic performance parameter of PSCs prepared based on PCBM:CY4 at different concentrations.

Concentration (mg mL ⁻¹)	J_{SC} (mA cm ⁻²)	V_{OC} (V)	FF (%)	PCE (%)
Control	21.59	1.03	77.06	17.20
0.01	22.46	1.06	79.16	18.85
0.02	22.89	1.08	80.11	19.80
0.04	22.38	1.05	77.87	18.30
0.06	21.07	1.04	75.17	16.47
0.1	20.04	1.01	70.81	14.33

Table S4. Summary of work for p-i-n type PSCs with PCBM as ETL and modified with additives in recent years.

ETL materials	PCE (%)	Ref.
PCBM:HRhMOP	18.64	J. Mater. Chem. C (2022) ^[S1]
PCBM:APTS	18.62	Sol. Energy Mater. Sol. Cells (2022) ^[S2]
PCBM:CBN	20.19	Small (2023) ^[S3]
PCBM:AZO	18.63	ChemNanoMat (2023) ^[S4]
PCBM:GF	20.80	J. Mater. Chem. A (2023) ^[S5]
PCBM:ZnO	17.97	Materials (2024) ^[S6]
PCBM:2,6-Lu	19.93	Surf. Interface (2024) ^[S7]
PCBM:CY3	18.78	This work
PCBM:CY4	19.80	This work

Reference:

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