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Interfacial Engineering via Inserting Functionalized Water-soluble Fullerene Derivative Interlayers for Enhancing Performance of Perovskite Solar Cells

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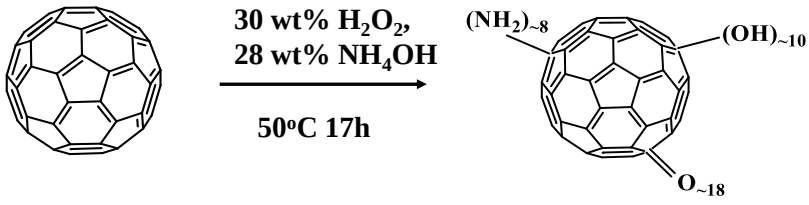
100 mg C_{60} or C_{70} was added to 9.84 mL of 30 wt % H_2O_2 and 7.2 mL of 28 wt % aqueous ammonia. The suspension was vigorously stirred at 50 °C under ambient conditions for 17h. At the end of the reaction, the black suspension was gradually dissolved. The mixtures turned into a yellow solution with some insolubles. After filtration with 0.45 um filter membrane, a transparent yellow solution was obtained. The remaining solution was concentrated to 3 mL, and then 30 mL anhydrous ethanol was added into the solution to produce a yellowish product and remove the excess H_2O_2 and NH_4OH. The precipitate was washed 3 times with anhydrous ethanol and then dried in vacuum oven at 40 °C for 12h.



C_{60} **Functionalized C_{60} (f-C_{60})**

Scheme S1. Synthetic route of f-C_{60}.

Table S1. Fitting of C_{1s} binding energy of C_{60} derivative

Bond (C_{1s})	Binding Energy (eV)	Area	FWHM (eV)
C-C, C=C	285.68	33564.11	1.56
C-O, C-N	287.40	22529.06	1.23
C=O	289.04	23803.61	1.78

Table S2. Fitting of N_{1s} binding energy of C_{60} derivative

Bond (N_{1s})	Binding Energy (eV)	Area	FWHM (eV)
$-NH_2$	400.38	10694.58	1.77
$-NH_3^+$	402.16	6326.69	1.51

Table S3. Curve fit results of C_{1s} binding energy of C_{70} derivative

Bond (C_{1s})	Binding Energy (eV)	Area	FWHM (eV)
C-C, C=C	285.25	41926.39	1.40
C-O, C-N	287.05	22729.48	1.46
C=O	288.85	21689.78	1.59

Table S4. Curve fit results of N_{1s} binding energy of C_{70} derivative

Bond (N_{1s})	Binding Energy (eV)	Area	FWHM (eV)
$-NH_2$	400.05	10765.35	1.72
$-NH_3^+$	401.84	8953.82	1.57

The percentage of C=O group of C_{60} derivative is 29.79 %, which means there are 18 C=O groups on the C_{60} carbon cage. Combined with C_{1s}/N_{1s} integration area and their sensitive factor (C_{1s} = 0.30, N_{1s} = 0.48), the average molecular formula can be designed as $C_{60}O_{\sim 18}(OH)_{\sim 10}(NH_2)_{\sim 8}$. According to the same rule, the average molecular formula of C_{70} derivative can be designed as $C_{70}O_{\sim 18}(OH)_{\sim 10}(NH_2)_{\sim 10}$.

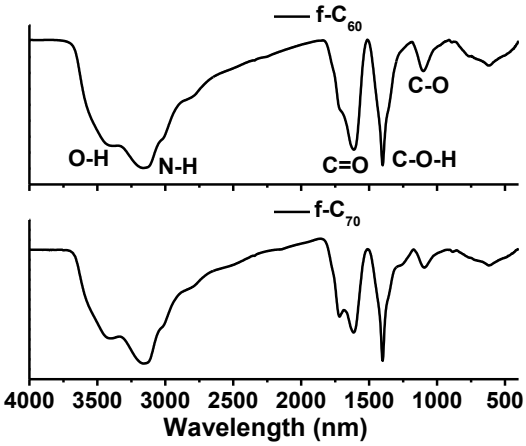


Figure S1. FT-IR spectra of f-C_{60} and f-C_{70}.

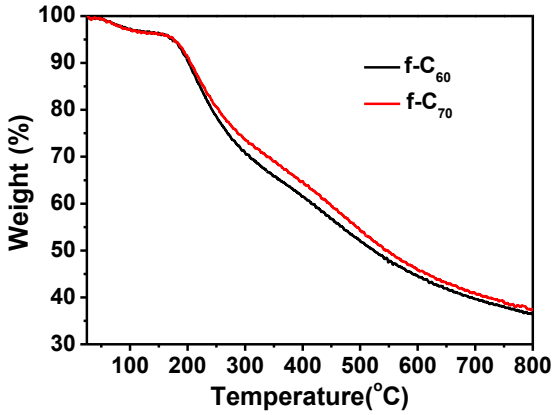


Figure S2. TGA curves of f-C_{60} and f-C_{70}.

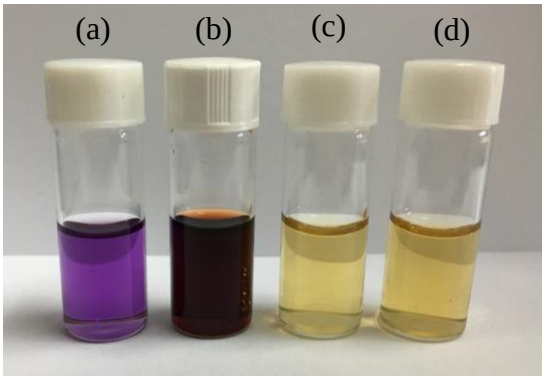


Figure S3. (a) 0.5mg/mL C_{60} and (b) 0.5 mg/mL C_{70} in toluene, (c) 0.5mg/mL f-C_{60} and (d) 0.5mg/mL f-C_{70} in ultrapure water.

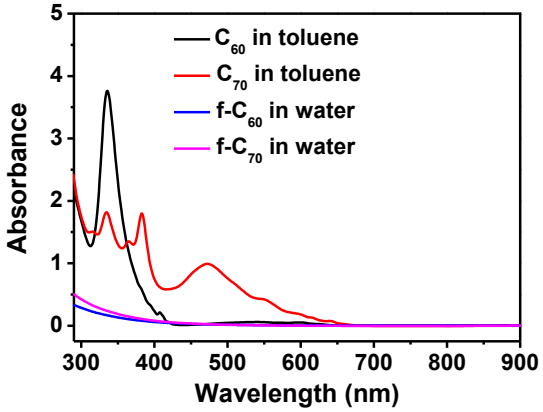


Figure S4. UV-vis absorption spectra of C_{60} and C_{70} in toluene, f-C_{60} and f-C_{70} in water, all the concentration of the samples are 0.05mg/mL.

Table S5. Summary of the photovoltaic parameters of the Pero-SCs with pristine f-C_{60} and f-C_{70} only as ETL

ETL	Concentration (mg/mL)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
/	/	0.92	11.24	39.92	4.15
f-C_{60}	0.3	0.95	13.35	43.52	5.53
	0.5	0.99	13.39	58.63	7.78
	0.75	0.97	17.83	37.39	6.44
	1	0.86	14.91	38.30	4.91
f-C_{70}	0.3	0.96	14.08	39.84	5.41
	0.5	0.98	15.21	48.03	7.14
	0.75	0.91	16.74	37.09	5.63
	1	0.92	13.85	33.51	4.27

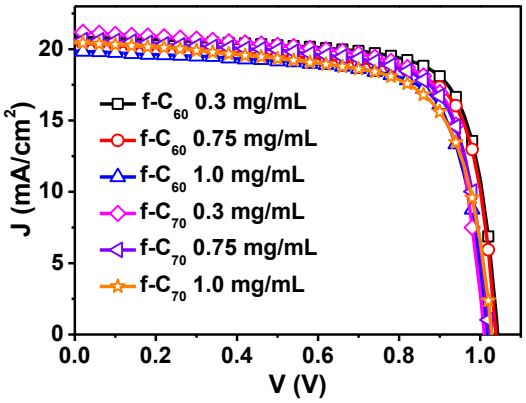


Figure S5. *J*-*V* curves of devices with different concentration of f-C_{60} and f-C_{70} ETL.

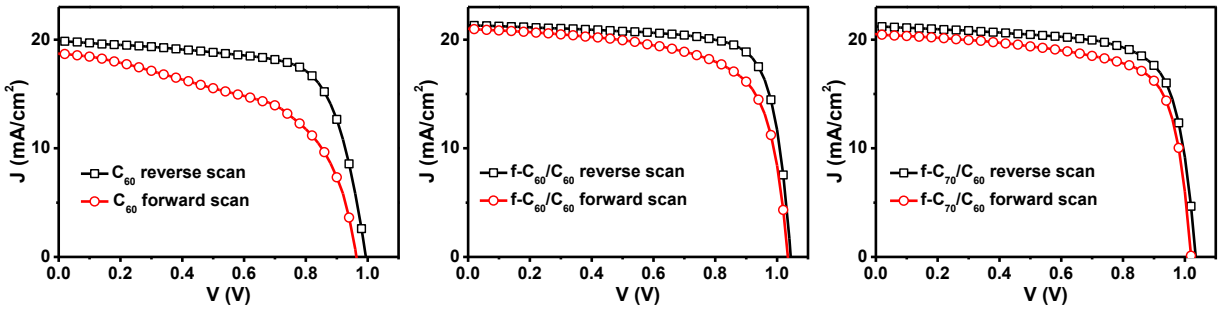


Figure S6. *J*–*V* characteristics with forward and reverse scans of the Pero-SCs based on C_{60}, f-C_{60}/C_{60} and f-C_{70}/C_{60} ETL.

Table S6. The photovoltaic parameters of Pero-SCs without and with f-C_{60} or f-C_{70} layer measured under reverse and forward voltage scanning.

	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
C_{60} Reserve Scan	0.99	19.87	69.38	13.71
C_{60} Forward Scan	0.96	18.71	54.47	9.82
f-C_{60}/C_{60} Reserve Scan	1.04	21.32	76.25	16.97
f-C_{60}/C_{60} Forward Scan	1.03	21.01	67.47	14.67
f-C_{70}/C_{60} Reserve Scan	1.03	21.21	72.58	15.94
f-C_{70}/C_{60} Forward Scan	1.02	20.51	70.39	14.73

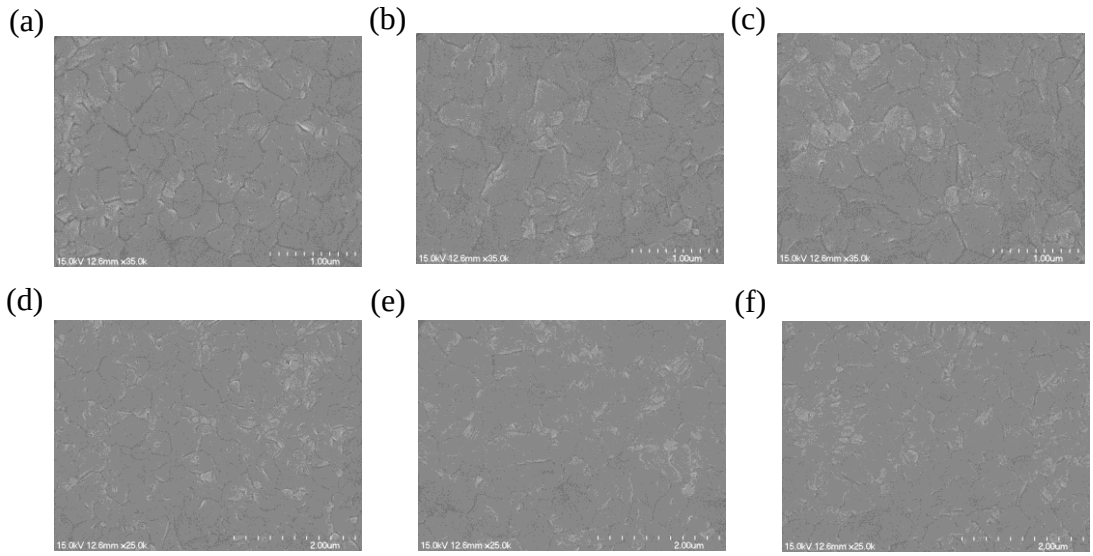


Figure S7. Top-view SEM images of perovskite layer on (a) and (d) pristine C_{60}, (b) and (e) f-C_{60}/C_{60} layer, (c) and (f) f-C_{70}/C_{60} layer

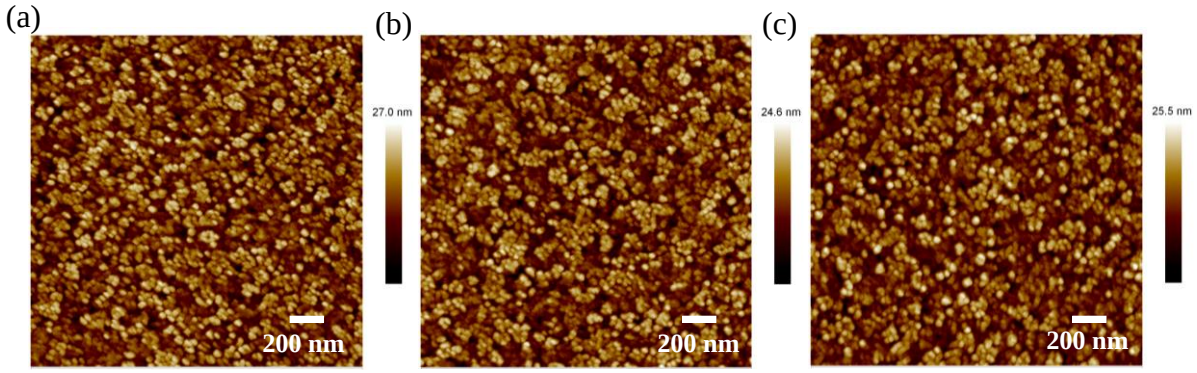


Figure S8. AFM images of (a) ITO/C_{60}, (b) ITO/f-C_{60}/C_{60}, and (c) ITO/f-C_{70}/C_{60}.