



Supporting Information

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High-Efficiency Fullerene Solar Cells Enabled by a Spontaneously Formed Mesostructured CuSCN-Nanowire Heterointerface

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High efficiency fullerene solar cells enabled by a spontaneously formed mesostructured CuSCN-nanowire heterointerface

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Table S1. Summary of the mean extracted parameters from bilayer and mixed layer cells under AM1.5 illumination. The values for the best cell are given in brackets.

	V_{oc} [V]	J_{sc} [mA cm ⁻²]	FF [%]	PCE [%]
PC ₇₀ BM/CuSCN (bilayer)	0.98 ± 0.030 (0.95)	1.8 ± 0.24 (2.2)	48 ± 3.2 (49)	0.84 ± 0.12 (1.0)
PC ₇₀ BM:CuSCN (mixed layer)	0.91 ± 0.005 (0.91)	7.9 ± 0.11 (8.3)	71 ± 1.9 (72)	5.10 ± 0.17 (5.4)

Table S2. Solar cell performance dependence on the PC₇₀BM thickness for bilayer cells (top table) and the performance dependence on the CuSCN:PC₇₀BM ratio of mixed layer cells for two different total solid concentrations (bottom table).

Active layer	V_{oc} [V]	J_{sc} [mA cm ⁻²]	FF [%]	PCE [%]	
CuSCN/PC ₇₀ BM (bilayer)					
30 nm	0.98 ± 0.03	1.8 ± 0.24	48 ± 3.2	0.84 ± 0.12	
50 nm	0.96 ± 0.01	1.7 ± 0.01	43 ± 1.0	0.70 ± 0.03	
85 nm	0.94 ± 0.02	0.5 ± 0.09	39 ± 2.3	0.18 ± 0.04	
105 nm	0.93 ± 0.02	0.36 ± 0.05	40 ± 5.3	0.13 ± 0.04	
CuSCN:PC ₇₀ BM (mixed layer)					
Total solid: 25 mg/ml	1:5	0.93 ± 0.004	5.9 ± 0.15	71 ± 1.6	3.9 ± 0.15
	1:3	0.92 ± 0.007	7.1 ± 0.06	73 ± 0.9	4.7 ± 0.07
	1:2	0.92 ± 0.004	7.6 ± 0.12	72 ± 1.7	5.0 ± 0.08
Total solid: 40 mg/ml	1:5	0.92 ± 0.008	7.0 ± 0.11	71 ± 1.2	4.6 ± 0.12
	1:3	0.91 ± 0.005	7.9 ± 0.11	71 ± 1.9	5.1 ± 0.17
	1:2	0.92 ± 0.008	7.9 ± 0.08	67 ± 3.1	4.8 ± 0.16

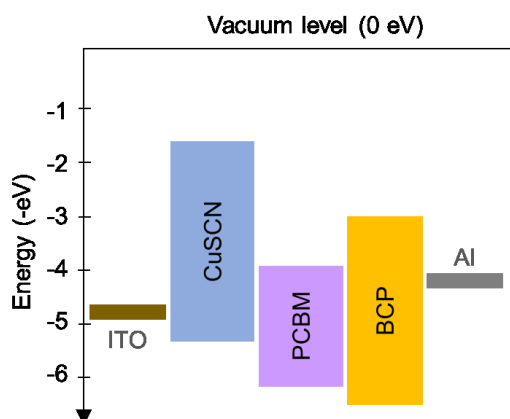


Figure S1. Energy levels of the various materials used to fabricate solar cells.

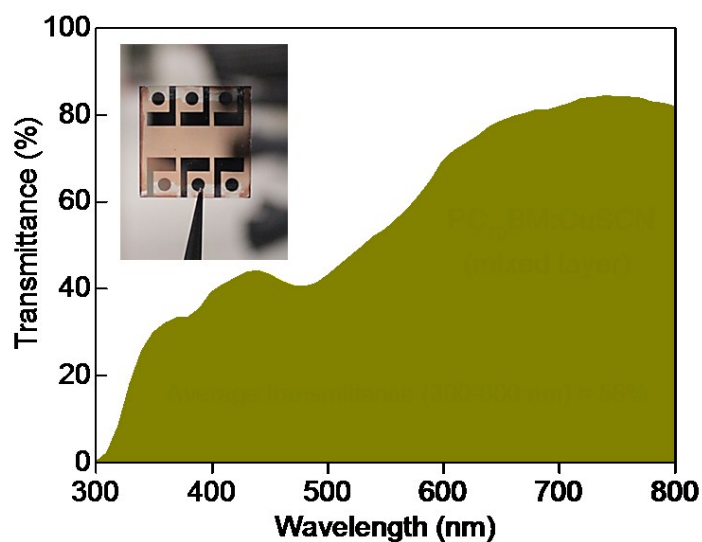


Figure S2. Transmission spectra of an optimized CuSCN:PC₇₀BM mixed layer device measured without the top Al electrode. The active layer of the device exhibits an average transmittance between 300-800 nm of 56%. Inset: photograph of the actual device.

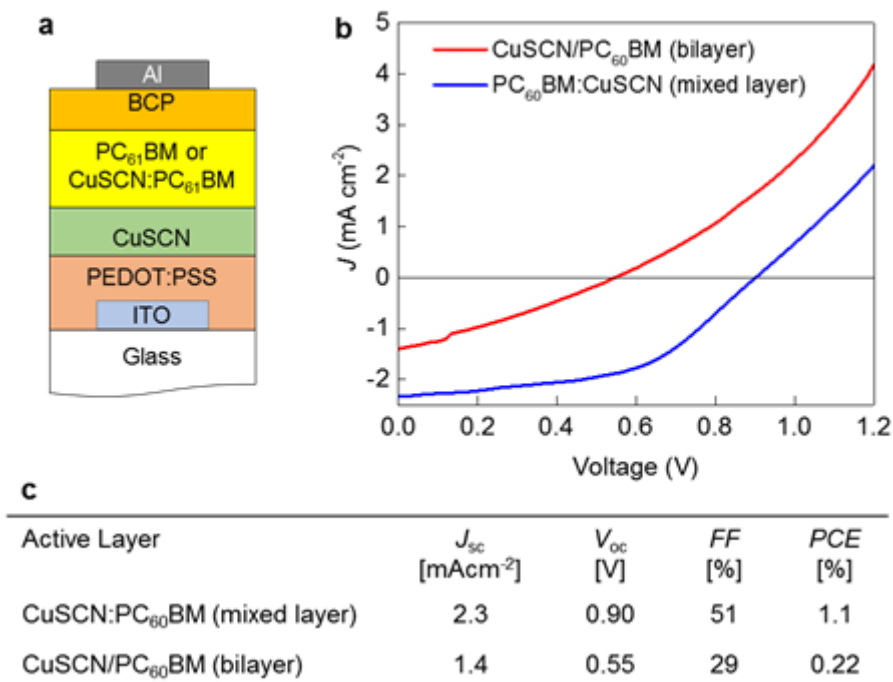


Figure S3. (a) Device architecture of the CuSCN:PC₆₀BM solar cells. (b) J - V characteristics measured for a CuSCN/PC₆₀BM bilayer and a CuSCN:PC₆₀BM mixed layer solar cells. (c) Summary of key device parameters extracted from the J - V characteristics.

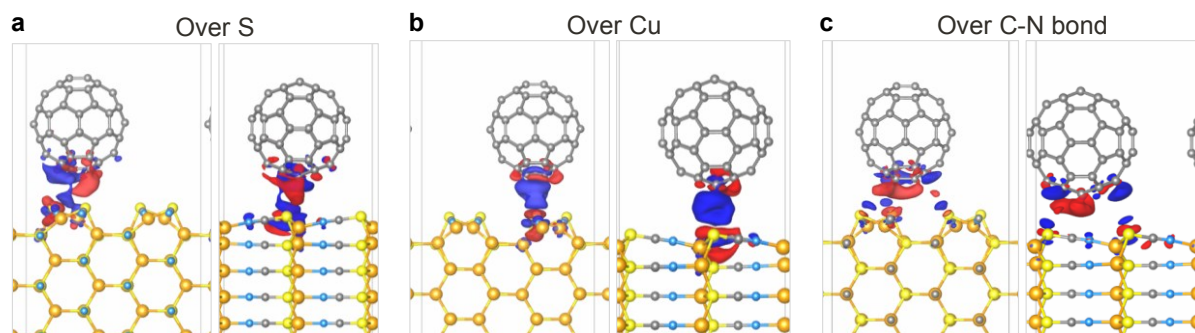


Figure S4. Atomistic model and charge density re-arrangement of the adsorption of a C₆₀ molecule onto CuSCN viewed from the top (left) and side on (right) over three different possible adsorption sites: a) over a surface S atom, (b) over a Cu atom and (c) over the C-N bond. The calculated adsorption energies are almost the same for all three sites. Blue (red) shows the positive (negative) charge redistribution upon absorption of the C₆₀.

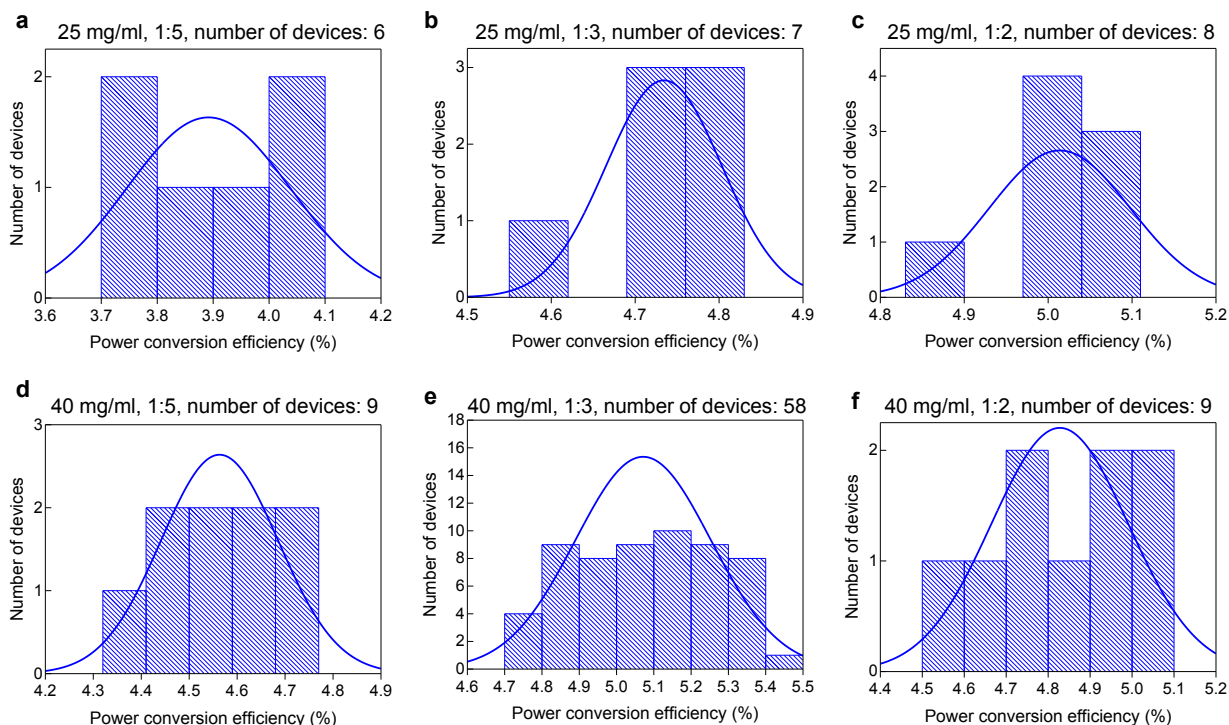


Figure S5. (a-f) Plots of the statistical device power conversion efficiency (PCE) versus number of devices for the data of the mixed-layer cells of different CuSCN:PCBM compositions corresponding to the values shown in Table S2 (bottom). The total solid concentration, followed by the ratio of CuSCN to PC₇₀BM content and the total number of devices tested are indicated above each plot.

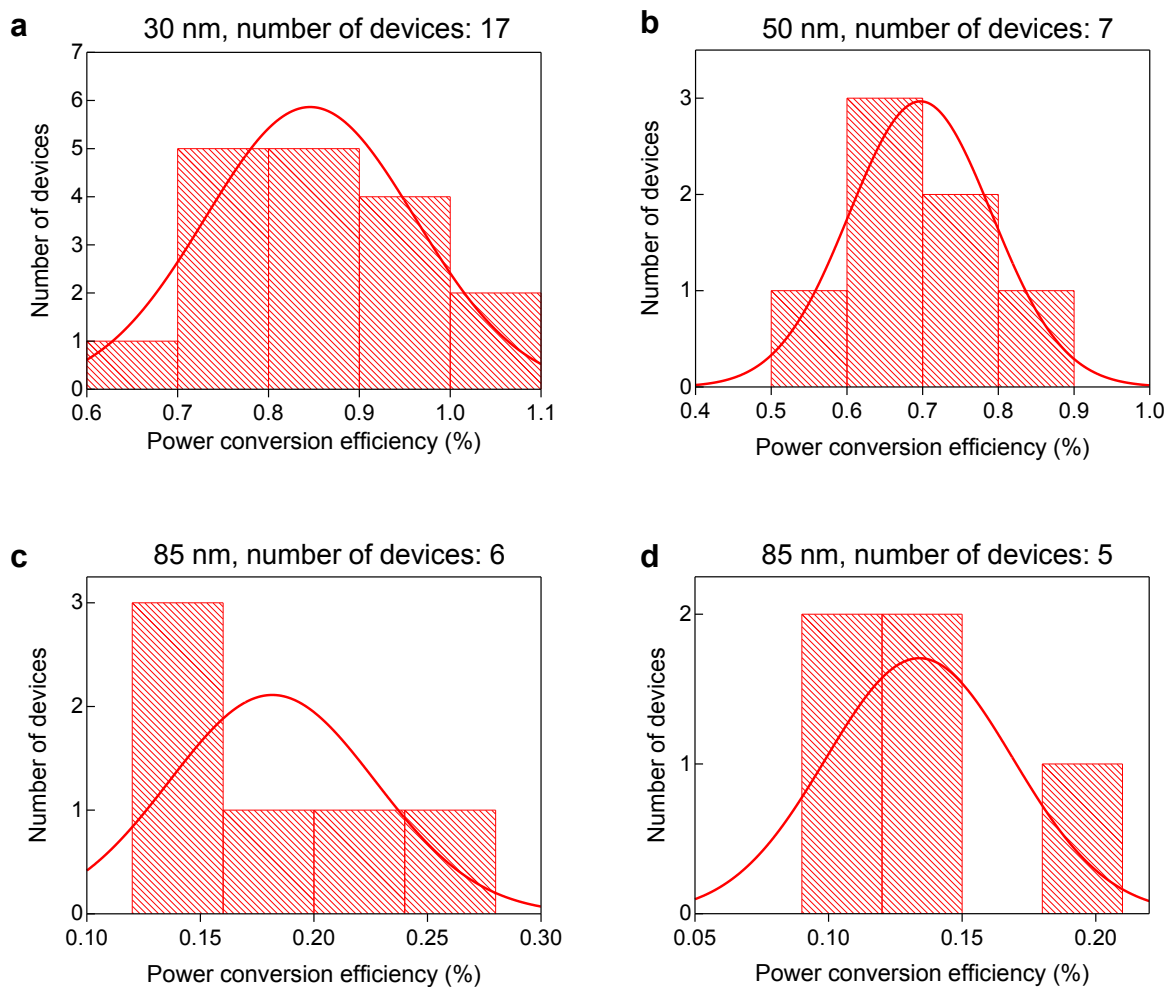


Figure S6. (a-d) Plots of the statistical device power conversion efficiency (PCE) versus number of devices for the data of the bilayer cells of different thicknesses corresponding to the values shown in Table S2 (top). The PC₇₀BM thickness followed by the total number of devices tested is indicated above each plot.