

Supporting information

Cu₃PS₄ Nanoparticle Hole Selective Layer for Efficient Inverted Perovskite Solar Cells

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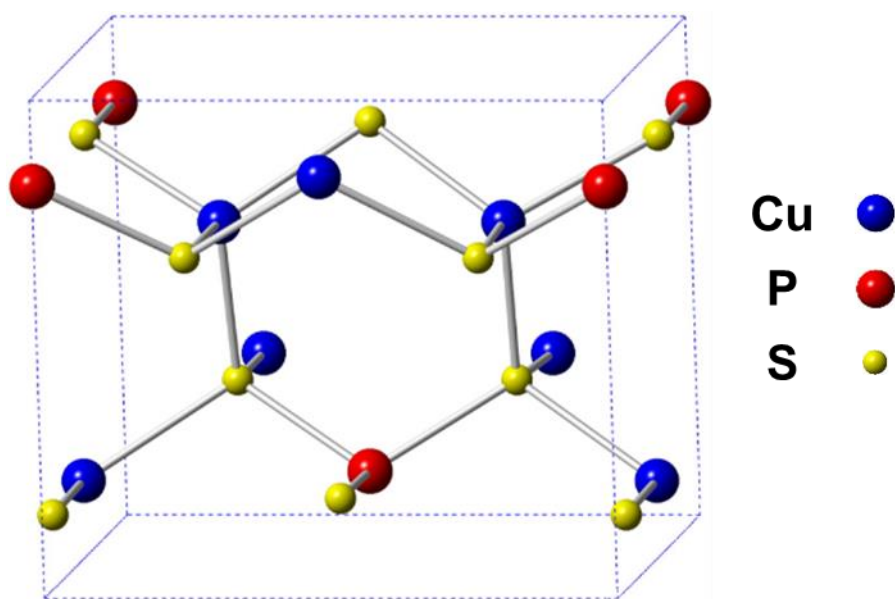


Figure S1. Unit cell of Cu_3PS_4 . The wurtzite-derived enargite structure (space group $Pmn2_1$) is adopted.

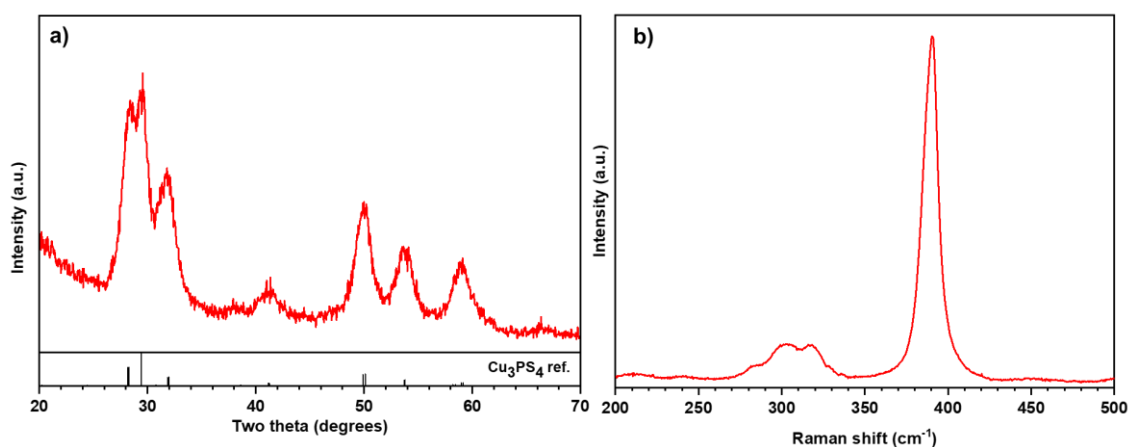


Figure S2. a) XRD and b) Raman spectra of as-synthesized Cu_3PS_4 nanoparticles. The peaks in the XRD spectra match with reference standard JCPDS 01-071-3306, and the Raman spectra matches with a previous reference.¹

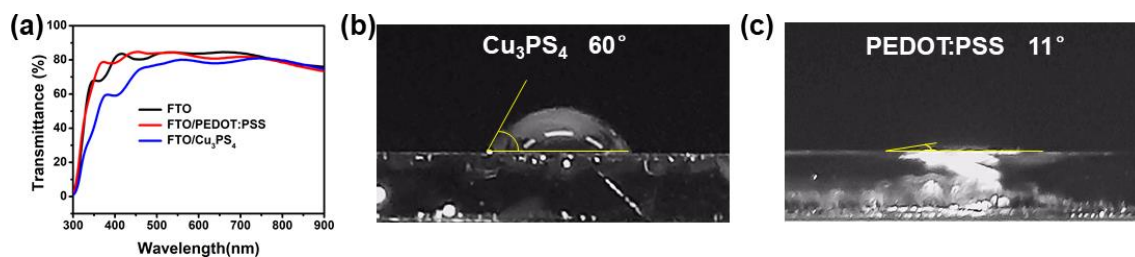


Figure S3. (a) The optical transmission spectra of bare FTO glass and PEDOT:PSS or Cu_3PS_4 film on FTO. Contact angle measurement of water droplet on the surface of (b) Cu_3PS_4 and (c) PEDOT:PSS.

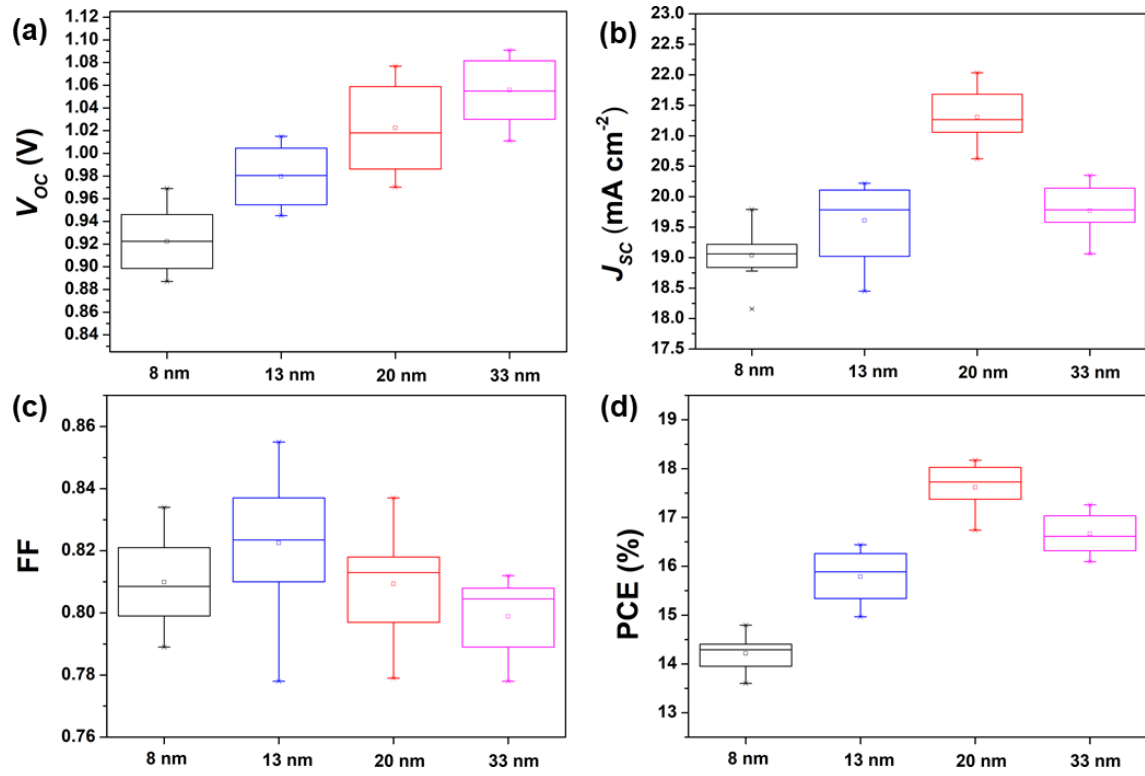


Figure S4. Photovoltaic parameters of PSCs with different Cu_3PS_4 thicknesses. Histograms of (a) V_{OC} , (b) J_{SC} , (c) FF, and (d) PCE of corresponding devices.

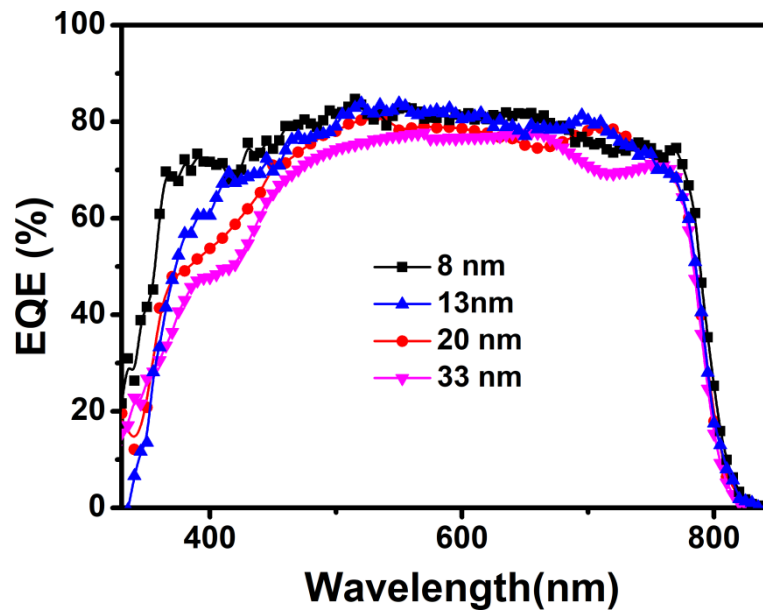


Figure S5. EQE spectra of PSCs with different thicknesses of Cu_3PS_4 .

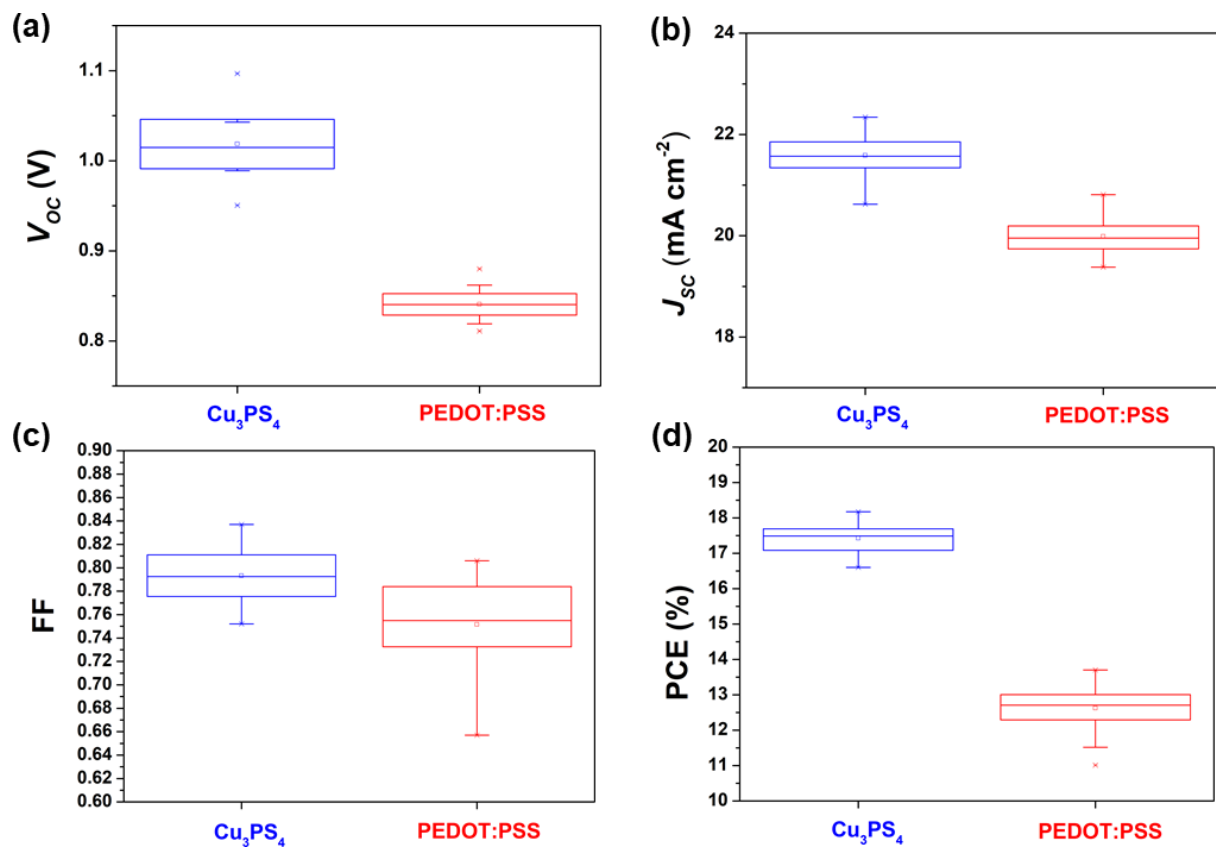


Figure S6. Photovoltaic parameters of PSCs with 20 nm Cu_3PS_4 or PEDOT:PSS HSL. Histograms of (a) V_{oc} , (b) J_{sc} , (c) FF, and (d) PCE of corresponding devices.

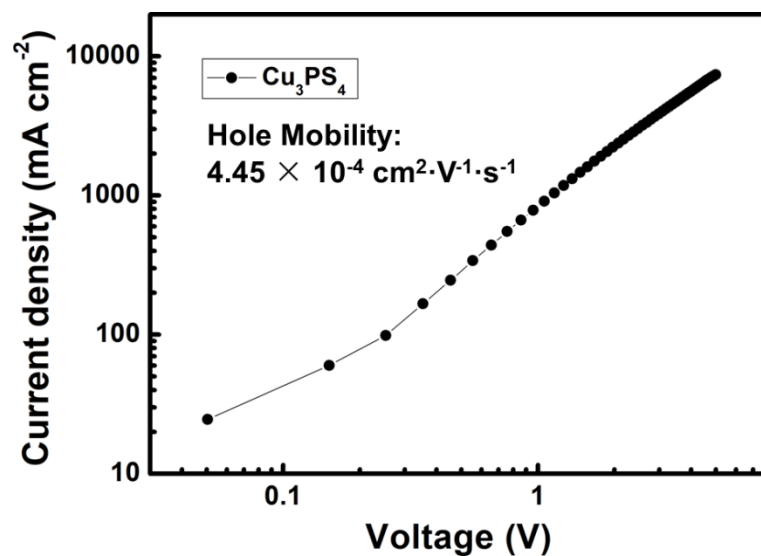


Figure S7. Space-charge-limited current (SCLC) J - V characteristics of Cu_3PS_4 -based hole-only devices.

Table S1. Summary of photovoltaic performance of Cu-based HSL materials for p-i-n perovskite solar cells.

HSL	Effective mass of holes (m_0)	Bandgap (eV)	J_{SC} (mA cm^{-2})	V_{OC} (V)	FF	PCE (%)	Reference
CuI	1.4 ²	3.1	22.80	1.01	0.730	16.8	3
Cu ₂ O	1.3 ⁴	2.1	16.52	1.07	0.755	13.4	5
CuO	3.5 ⁴	1.3	15.82	1.06	0.725	12.2	5
CuO _x	--	2.0	22.50	1.11	0.758	19.0	6
CuS	--	2.2	22.30	1.02	0.712	16.2	7
CuSCN	1.5 ⁸	3.6	22.30	1.09	0.710	17.2	9
CuCrO ₂	3.6 ⁴	2.9	21.94	1.07	0.810	19.0	10
CuInS ₂	2.87 ¹¹	1.5	23.80	0.95	0.730	16.5	12
Cu₃PS₄	0.8	2.2	20.83	1.07	0.816	18.2	This work

Table S2. Spin-coating parameters for achieving Cu₃PS₄ layer with different thicknesses.

Cu ₃ PS ₄ Thickness (nm)	Solution Concentration mg/mL	Speed rpm
8	10	4000
13	17	4000
20	30	4000
33	40	2000

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