Supporting Information

Solution-Processed, Inverted $AgBiS_2$ Nanocrystal Solar Cells

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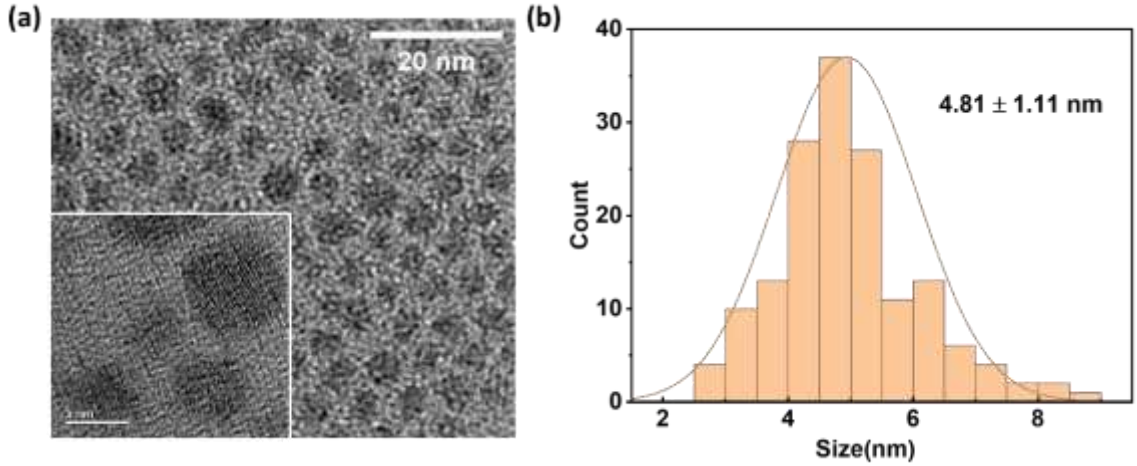

Figure S1: (a) HRTEM image of $AgBiS_2$ nanocrystals and (b) size distribution histogram.

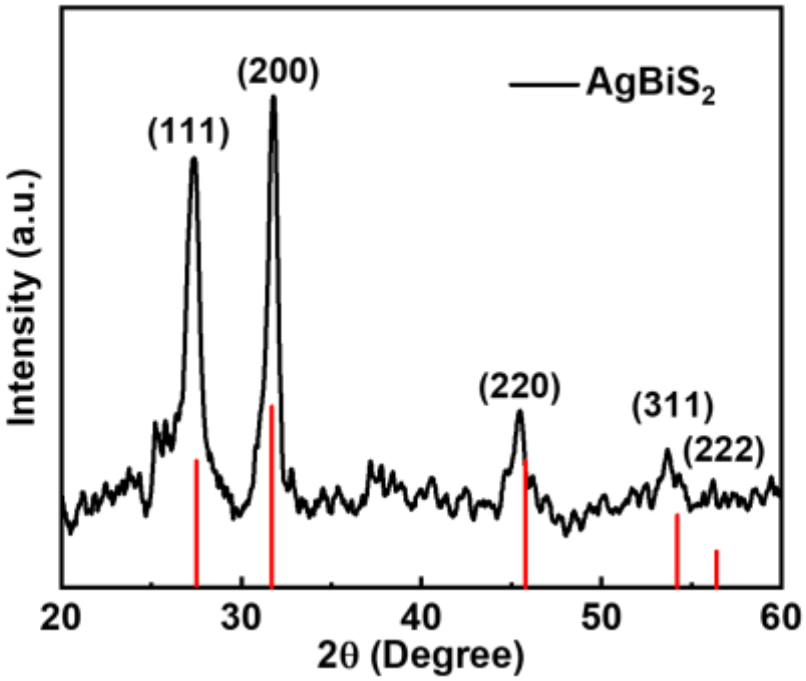

Figure S2: XRD pattern of $AgBiS_2$ NCs thin film. Red solid lines refer to PDF#21-1178.

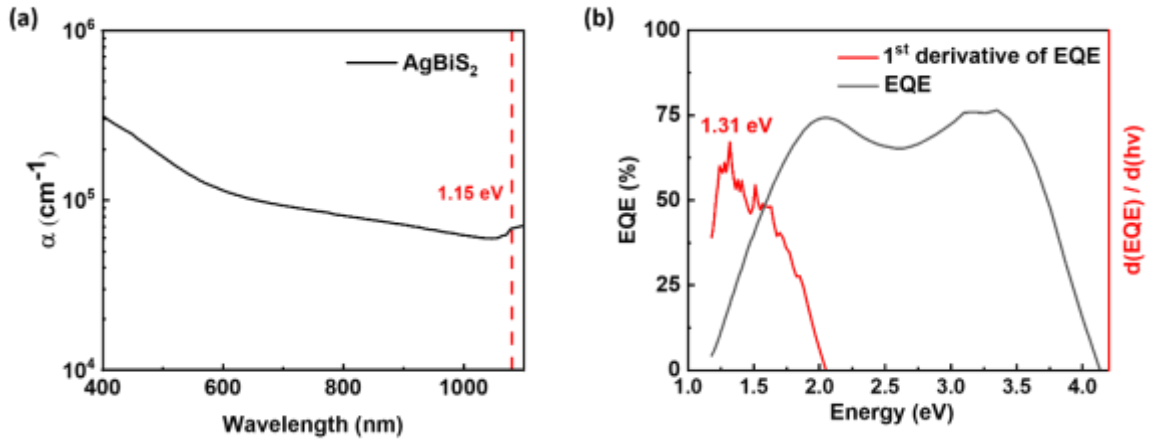

Figure S3: (a) Absorption coefficient measurement of 3 layers $AgBiS_2$ thin film on quartz. Methyl acetate was applied to wash the excess oleate ligands between each layer. (b) $AgBiS_2$ p-i-n devices EQE spectrum and the first derivative of EQE. The bandgap of $AgBiS_2$ is highlighted in red text.

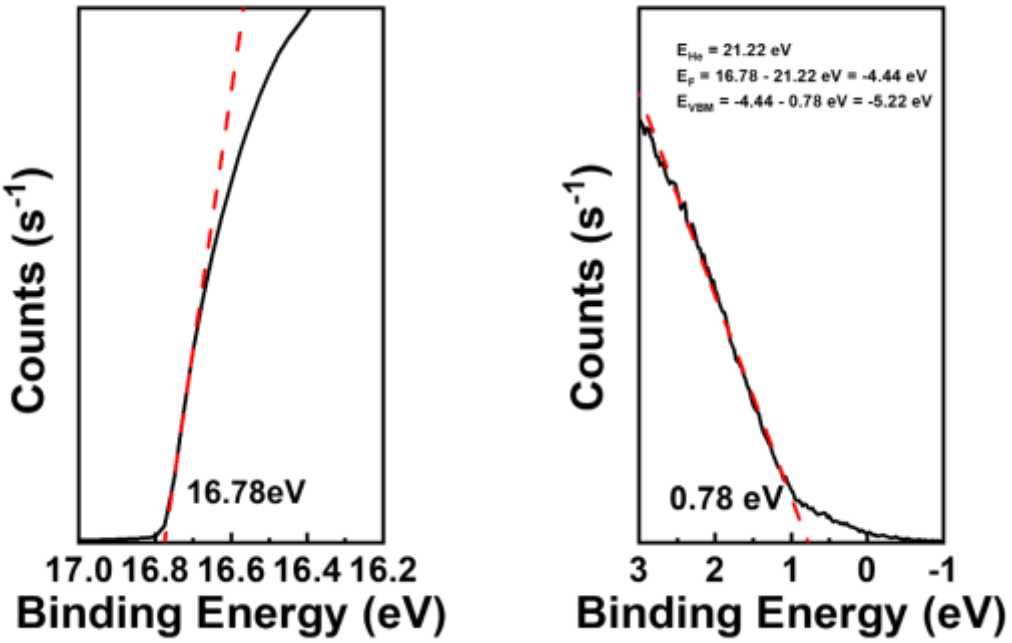

Figure S4: UPS (UV excitation by HeI at 21.22 eV) spectra of the $AgBiS_2$ film.

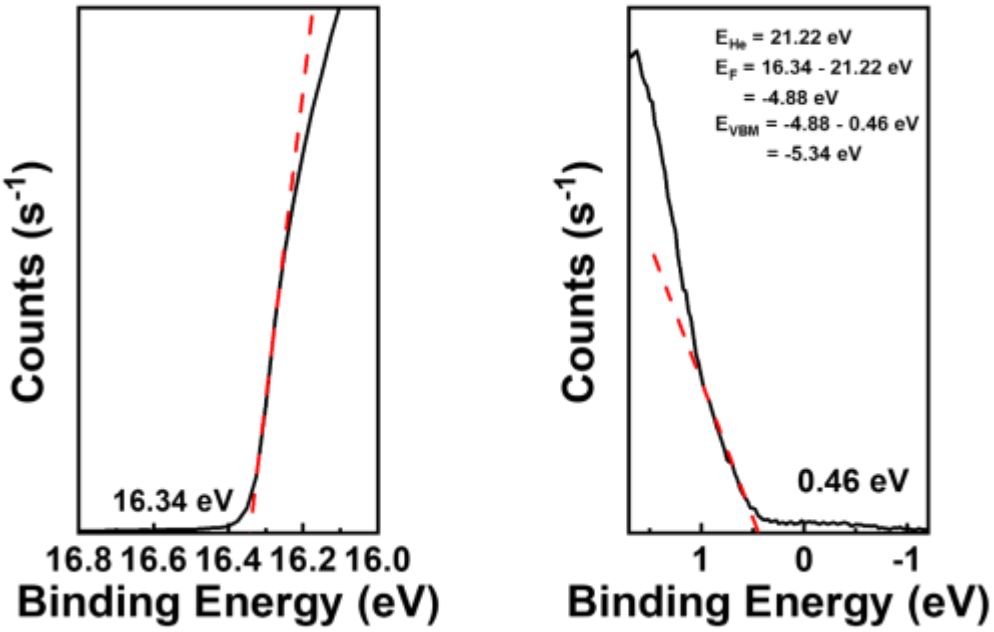

Figure S5: UPS (UV excitation by HeI at 21.22 eV) spectra of spray coated NiO film.

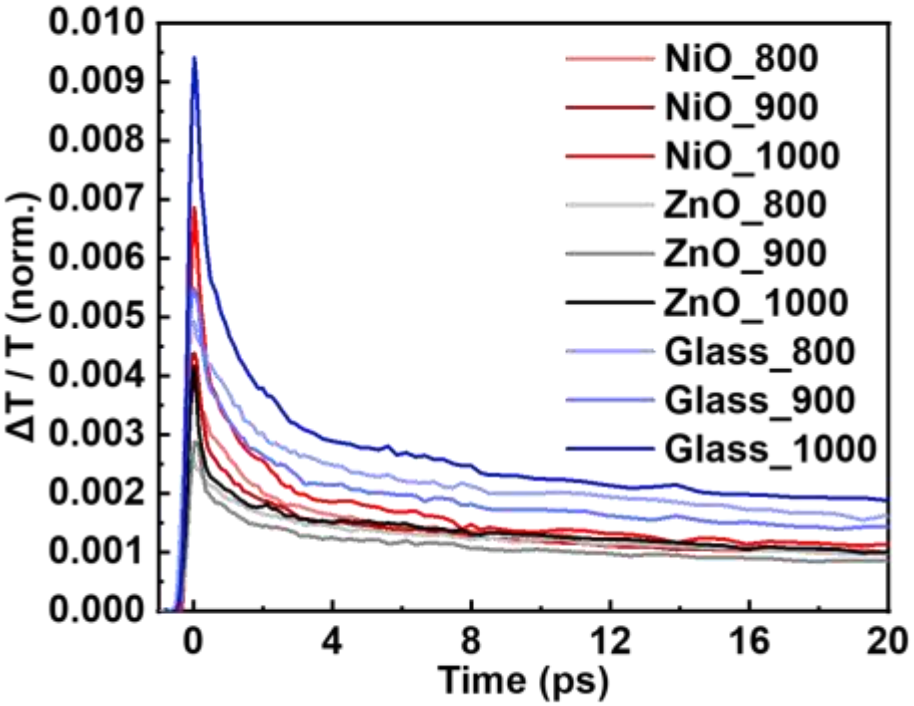

Figure S6: Transient absorption (TA) time profiles of $AgBiS_2$ nanocrystals on Glass / NiO / ZnO surface.

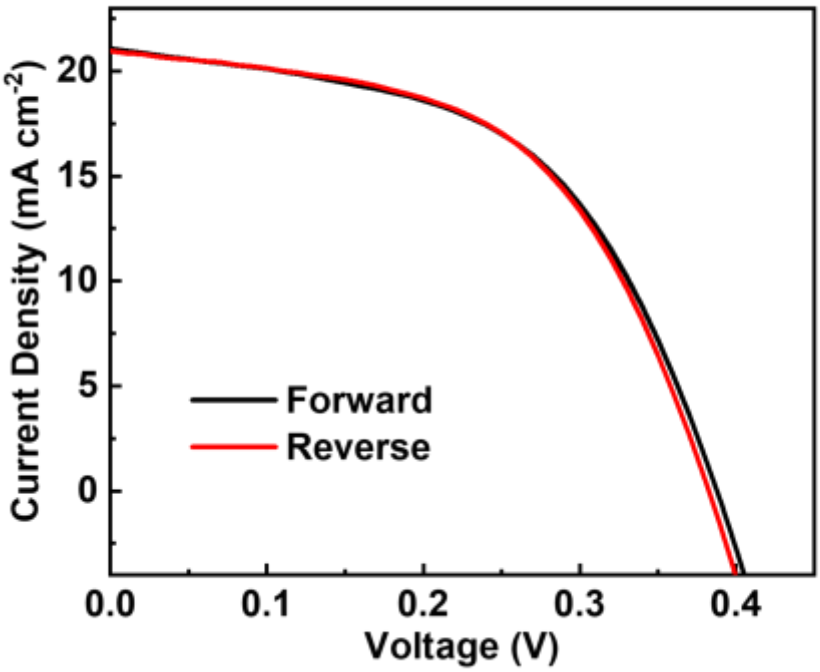

Figure S7: JV curve for forward and reverse scan for p-i-n $AgBiS_2$ solar cell (-0.2V – 0.7V, step ±0.01 V, rate 0.01s). No obvious hysteresis is observed.

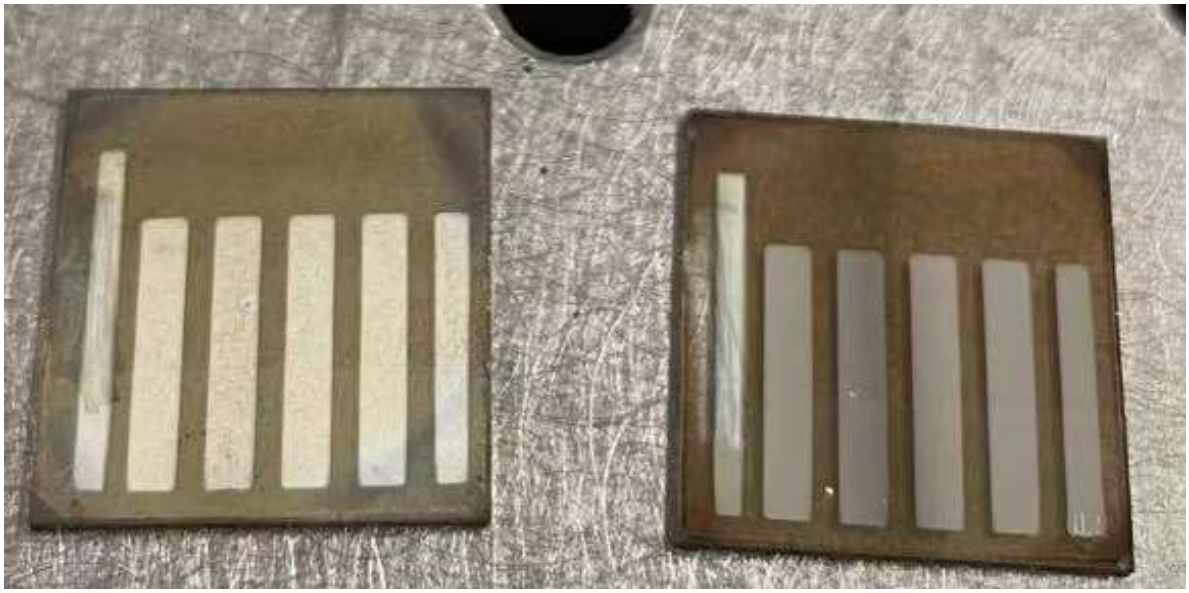

Figure S8: Picture of $AgBiS_2$ solar cells using different ETLs: C_{60} (left) and PCBM (right). The solar cell spin-coated with C_{60} in chlorobenzene shows rough film due to the low solubility of C_{60}.

Chemicals	Structure	Purity	Amount	Price (USD)	Amount used per 100 chips	Price per 100 chips
$Ni(acac)_2$	p-i-n HTL	96%	100 g	79	0.25 g	0.20 USD
ACN	p-i-n HTL	99.9%	4 L	96	100 mL	2.4 USD
PCBM	p-i-n ETL	99%	1 g	866	25 mg	21.6 USD
BCP	p-i-n ETL	99.99%	500 mg	225	5 mg	2.25 USD
Summary	p-i-n					26.45 USD
$Zn(OAc)_2$	n-i-p ETL	99%	250 g	87	0.5 g	0.17 USD
Ethanolamine	n-i-p ETL	98%	100 mL	39.4	1 mL	0.39 USD
PTB7	n-i-p HTL	99.9%	100 mg	656	25 mg	164 USD
MoO_x	n-i-p HTL	99.9%	5 g	82	5 mg	0.82 USD
Summary	n-i-p					165.38 USD

Table S1. Summary of the costs of p-i-n structure and n-i-p structure in USD. All the prices are obtained at: www.sigmaaldrich.com.

HTL	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF	PCE (%)
20 nm NiO	0.32	20.07	0.40	2.51
30 nm NiO	0.38	20.71	0.54	4.25
40 nm NiO	0.37	20.57	0.49	3.73
PEDOT:PSS	0.00	0.37	N/A	N/A
NiO Sol-gel (30 nm)	0.36	7.92	0.24	0.70

Table S2. Summary of inverted $AgBiS_2$ solar cells photovoltaic performances with different hole transporting layer (HTL). We also applied the NiO film by reported sol-gel method[S1], and compare the device performances. The sol-gel NiO shows a worse photovoltaic performance than the spray-coated NiO. We attributed such a decrease in PCE to the lower valence band energy (-5.7 eV, by UPS), which results in a poor hole transporting process.

Sample	Probe Wavelength (nm)	A_1	τ_1	A_2	τ_2	R^2
Glass_$AgBiS_2$	800	8.383	1.316	7.707	15.522	0.997
Glass_$AgBiS_2$	850	9.038	1.136	6.918	14.660	0.999
Glass_$AgBiS_2$	900	9.731	0.825	7.409	13.259	0.995
Glass_$AgBiS_2$	950	13.240	0.806	8.400	12.985	0.994
Glass_$AgBiS_2$	1000	19.630	0.793	10.632	12.656	0.994
ZnO_$AgBiS_2$	800	3.557	1.307	4.101	16.227	0.996
ZnO_$AgBiS_2$	850	4.290	1.041	4.022	13.519	0.993
ZnO_$AgBiS_2$	900	3.816	1.054	3.745	14.192	0.992
ZnO_$AgBiS_2$	950	4.822	0.894	4.376	13.689	0.988
ZnO_$AgBiS_2$	1000	4.221	0.940	4.608	14.027	0.983
NiO_$AgBiS_2$	800	8.003	1.872	4.935	21.063	0.996
NiO_$AgBiS_2$	850	6.879	2.030	4.542	23.146	0.994
NiO_$AgBiS_2$	900	6.282	2.361	4.003	23.111	0.994
NiO_$AgBiS_2$	950	27.153	1.919	4.794	25.896	0.994
NiO_$AgBiS_2$	1000	25.909	2.341	5.159	28.230	0.989

Table S3. Summary of fitting parameters of TA spectroscopy.

Measurements	Sample	A	τ	R^2
TPV	n-i-p	0.489	35.14	0.963
TPV	p-i-n	0.902	96.33	0.985
TPC	n-i-p	1.088	30.39	0.932
TPC	p-i-n	1.052	45.75	0.965

Table S4. Summary of fitting parameters of TPV and TPC.

PCBM conc. (mg / mL)	BCP conc. (mg / mL)	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF	PCE (%)
1	1	0.32	10.15	0.32	1.04
5	1	0.38	20.71	0.54	4.25
10	1	0.35	20.42	0.52	3.72
20	1	0.12	5.37	0.13	0.08
5	0.1	0.37	8.50	0.40	1.26
5	0.5	0.40	21.18	0.50	4.23
5 (not annealed)	1	0.40	16.58	0.35	2.33
5	5	0.38	1.21	0.10	0.05

Table S5. Summary of the inverted $AgBiS_2$ solar cells photovoltaic performances with different concentration of PCBM / BCP.

REFERENCE

S1. Shivarudraiah, S. B.; Ng, M.; Li, C.-H. A.; Halpert, J. E. All-Inorganic, Solution-Processed, Inverted $CsPbI_3$ Quantum Dot Solar Cells with a PCE of 13.1% Achieved via a Layer-by-Layer FAI Treatment. *ACS Appl. Energy Mater.* **2020***, 3*, 5620-5627.