Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Encapsulating CoS_2-$CoSe_2$ heterostructured nanocrystals in N-doped carbon nanocubes as highly efficient counter electrode for dye-sensitized solar cells

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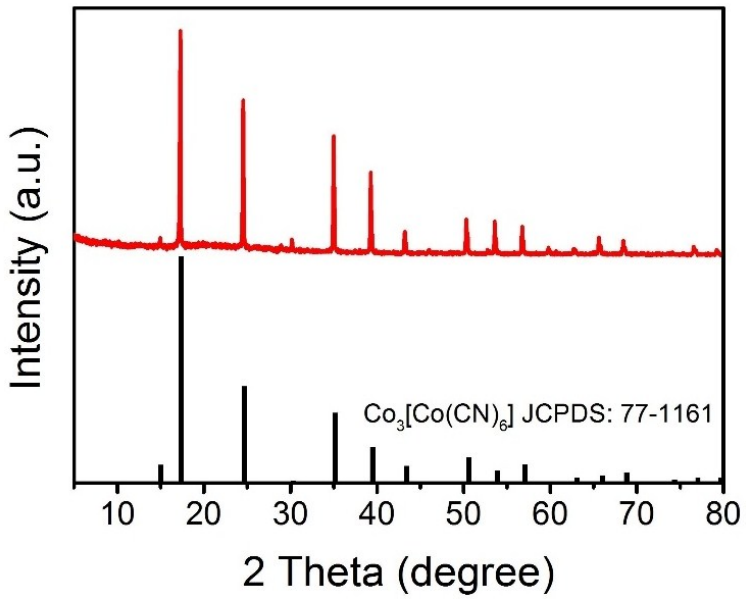

Fig. S1 XRD pattern of the as-synthesized $Co_3[Co(CN)_6]_2$ PBA nanocubes.

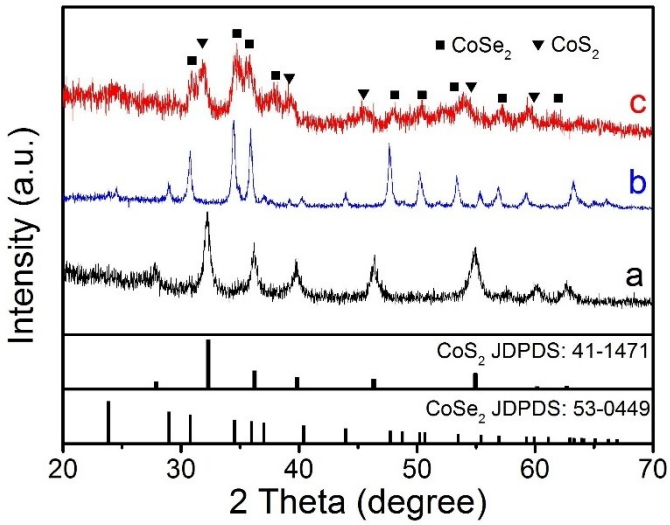

Fig. S2 XRD pattern of the as-prepared CoS_2@NC (a), $CoSe_2$@NC (b) and CoS_2-$CoSe_2$@NC (c) nanocubes.

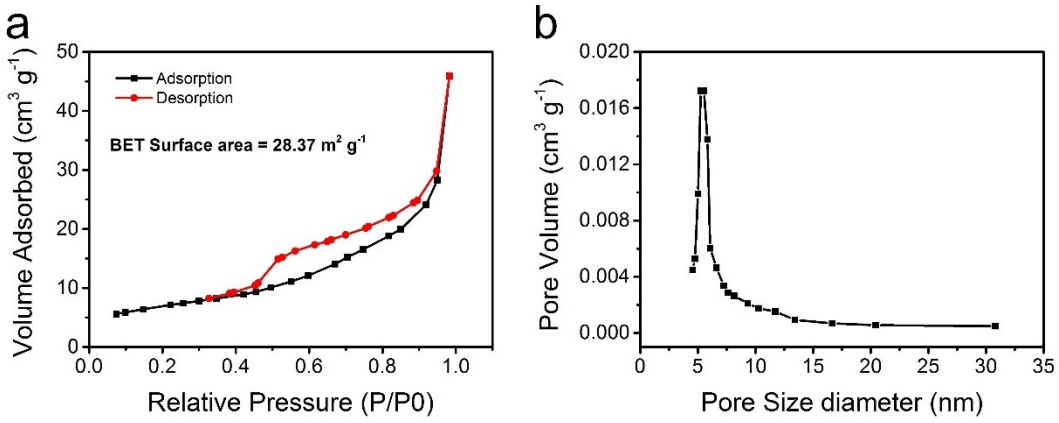

Fig. S3 Nitrogen adsorption/desorption isotherms (a) and pore size distribution of mesoporous CoS_2-$CoSe_2$@NC nanocubes (b).

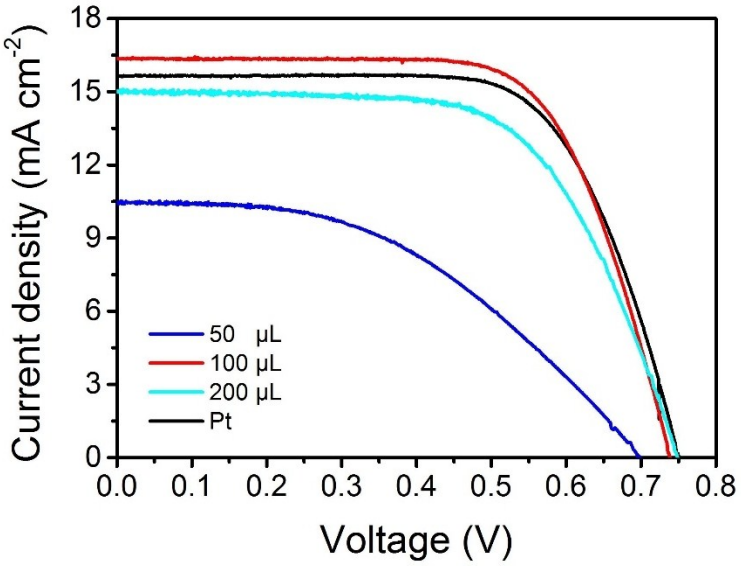

Fig. S4 J-V curve of DSSCs with different thickness of CoS_2-$CoSe_2$@NC and Pt CEs.

Tab. S1 Photovoltaic performance of DSSCs with different thickness of CoS_2-$CoSe_2$@NC and Pt CEs.

CEs	V_{oc} [mV]	J_{sc} [mA/cm^2]	FF	η [%]
50 µL	0.697 ± 0.006	10.42 ± 0.15	0.49 ± 0.02	3.56 ± 0.14
100 µL	0.740 ± 0.005	16.35 ± 0.11	0.70 ± 0.01	8.45 ± 0.06
200 µL	0.748 ± 0.013	15.03 ± 0.10	0.64 ± 0.01	7.19 ± 0.11
Pt	0.749 ± 0.003	15.53 ± 0.12	0.69 ± 0.00	8.07 ± 0.07

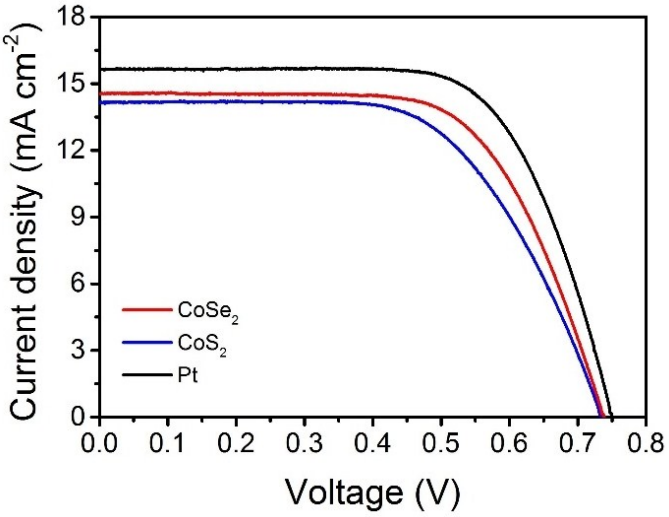

Fig. S5 J-V curves of the DSSCs with $CoSe_2$, CoS_2 and Pt CEs, measured under AM1.5G illumination (100 mW cm^{-2}).

Tab. S2 Photovoltaic performances of DSSCs with CoS_2, $CoSe_2$ and Pt CEs under AM1.5G illumination.

CEs	V_{oc} [V]	J_{sc} [mA/cm^2]	FF	η [%]
$CoSe_2$	0.736 ± 0.007	14.52 ± 0.15	0.65 ± 0.00	6.95 ± 0.13
CoS_2	0.732 ± 0.008	14.17 ± 0.09	0.63 ± 0.01	6.54 ± 0.08
Pt	0.749 ± 0.003	15.53 ± 0.12	0.69 ± 0.00	8.07 ± 0.07

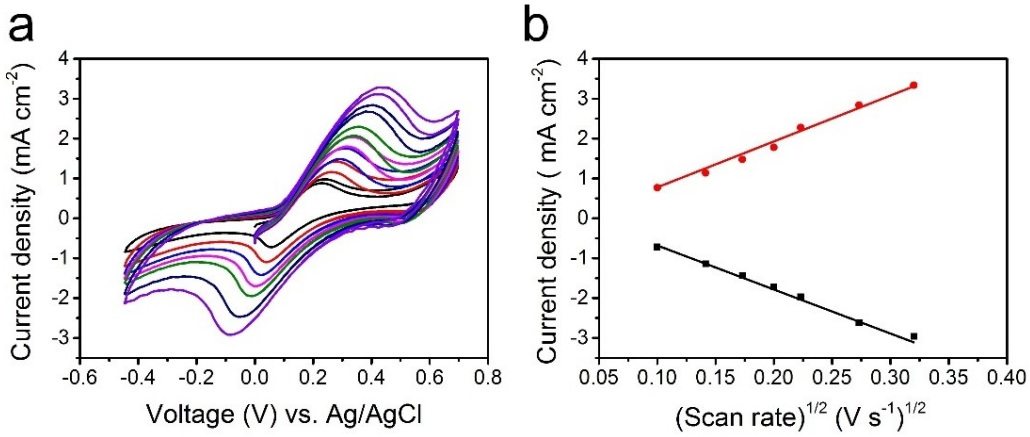

Fig. S6 (a) CV curves of the CoS_2-$CoSe_2$@NC nanocubes CE at different scan rate; (b) relationship between the peak current density and the square root of scanning rate of CoS_2-$CoSe_2$@NC nanocubes CEs.

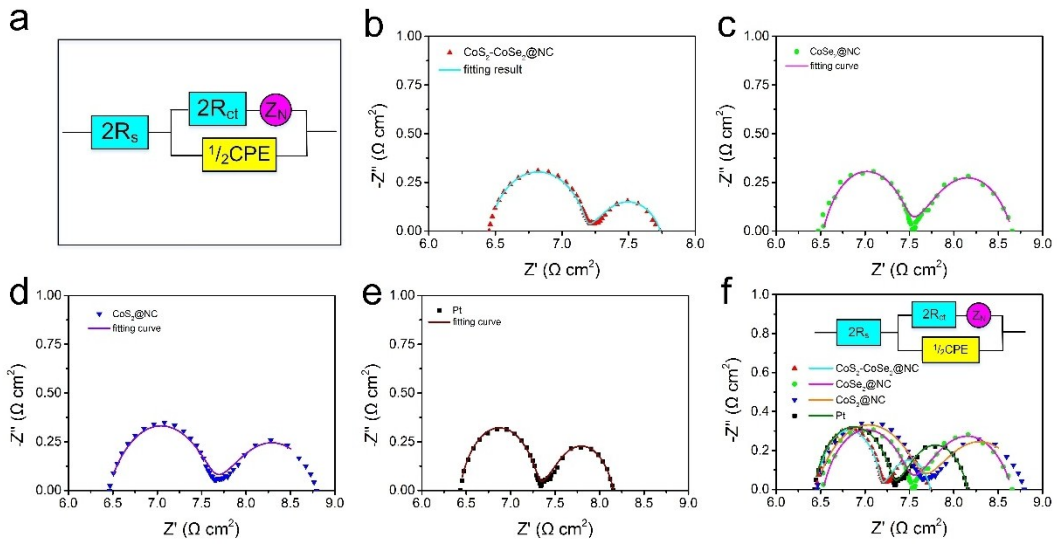

Fig. S7 The equivalent circuit diagram used to fit the impedance spectra in the symmetrical cells (a) and the fitting curves of CoS_2-$CoSe_2$@NC (a), $CoSe_2$@NC (b), CoS_2@NC (c) and Pt (d) CEs.

Tab. S3 Fitted electrochemical parameters from EIS.

CE	R_s Ω cm^2	R_{ct} Ω cm^2	CPE-T μF cm^{-2}	CPE-P	Ws-R Ω cm^2	Ws-T	Ws-P
CoS_2-$CoSe_2$@NC	3.23	0.38	269.16	0.84	0.54	0.35	0.50
$CoSe_2$@NC	3.26	0.51	220.52	0.83	1.10	0.68	0.50
CoS_2@NC	3.23	0.59	217.94	0.86	1.18	0.54	0.50
Pt	3.20	0.45	112.62	0.95	0.83	0.42	0.50

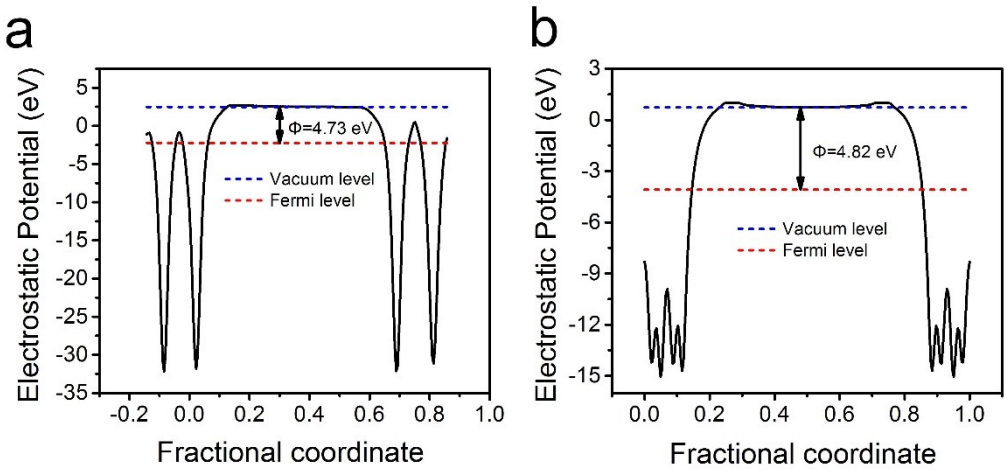

Fig. S8 Average potential profile along X-axis of (a) CoS_2 (001) and (b) $CoSe_2$ (100). The insert shows the calculated work function.

All of the density functional calculations were performed using the plane-wave pseudopotential method, implemented with the Cambridge Sequential Total Energy Package (CASTEP) code. The local density approximation (LDA) was used to describe the exchange-correlation effects. In order to obtain the work functions of CoS_2 and $CoSe_2$, two slab modules were created for the calculation. Both of the slabs consisted of a 30 Å vacuum layer and the surface cleaved for bulk material.[1-4] The atoms in the surface layer were fixed, while all other atoms were fully relaxed with force criteria of 0.025 eV/Å.

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2. Z. X. Qin, Y. B. Chen, Z. X. Huang, J. Z. Su, Z. D. Diao and L. J. Guo, *J. Phys. Chem. C*, 2016, **120**, 14581-14589.
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4. X. W. Wang, Y. Xie, B. Bateer, K. Pan, Y. T. Zhou, Y. Zhang, G. F. Wang, W. Zhou and H. G. Fu, *Nano Research*, 2016, **9**, 2862-2874.