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Electronic Supporting Information (ESI)

Zeolitic Imidazolate Framework-derived ZnSe/N-doped Carbon Cube Hybrid Electrocatalyst as the Counter Electrode for Dye-Sensitized Solar Cells

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Experimental section

Synthesis of ZIF-7

The ZIF-7 sample was synthesized according to the procedure reported previously[1]. Zinc nitrate hexahydrate (0.90 g, 3 mmol) was dissolved in ethanol (12.67 mL); benzimidazole (bIM, 0.72 g, 6 mmol) was dissolved in ethanol (38.02 mL), followed by the addition of ammonia hydroxide solution (3.18 mL, 48 mmol NH_3). The solution turned white immediately, and the resultant mixture was stirred for 10 min at room temperature to complete the crystallization. The product, ZIF-7, was collected by centrifugation and was washed with ethanol for three times, then dried at room temperature under atmosphere overnight.

Table S1 The performance of the reported DSSCs using various ZIF-derived CEs and ZnSe CEs, as compared to that obtained in this work.

Counter electrode	Metal	η (%)	η_{Pt} (%)	V_{OC} (V)	J_{SC} (mA cm^{-2})	*FF*	Ref.
ZIF-8 derived carbons[a]	Zn	7.32	7.53	0.77	13.56	0.68	2
ZIF-67 derived CoS_2[a] embedded carbon nanocages[a]	Co	8.20	7.88	0.73	16.90	0.66	3
ZIF-67 derived CoS[a]	Co	8.10	8.00	0.78	14.70	0.71	4
ZIF-67 derived carbons[a]	Co	7.92	8.18	0.80	13.29	0.74	5
ZnSe-10[b]		8.13	8.59	0.77	15.72	0.68	6
ZnSe/rGO[b]		6.61	6.23	0.78	15.00	0.57	7
$Cu_2ZnSnSe_4$[b]		8.22	7.56	N.A.	N.A.	N.A.	8
ZIF-7 derived ZnSe-NC[a]	Zn	8.69	8.26	0.77	16.40	0.69	This work

[a] ZIF-derived counter electrodes

[b] ZnSe counter electrodes (not derived from ZIFs)

Table S2 The photovoltaic parameters of the DSSCs with various CEs of ZIF-7, ZIF-NC, and ZIF-ZnSe-NC, measured at 100 mW cm^{-2}.

Samples[a]	η (%)	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF	k^0 (cm s^{-1})	A_e (cm^2)
ZIF-7	5.27 ± 0.08	0.77 ± 0.00	11.81 ± 0.36	0.58 ± 0.01	9.40×10^{-4}	0.405
ZIF-NC	6.02 ± 0.03	0.74 ± 0.00	12.27 ± 0.29	0.66 ± 0.01	1.30×10^{-3}	0.358
ZIF-ZnSe-NC	7.11 ± 0.04	0.76 ± 0.00	13.60 ± 0.19	0.69 ± 0.01	3.42×10^{-3}	0.805

[a] Average values and standard deviations were obtained from three independent cells.

Table S3 The photovoltaic parameters of the DSSCs with ZIF-ZnSe-NC CEs under different slurry concentrations (5~13 wt%), measured at 100 mW cm^{-2}.

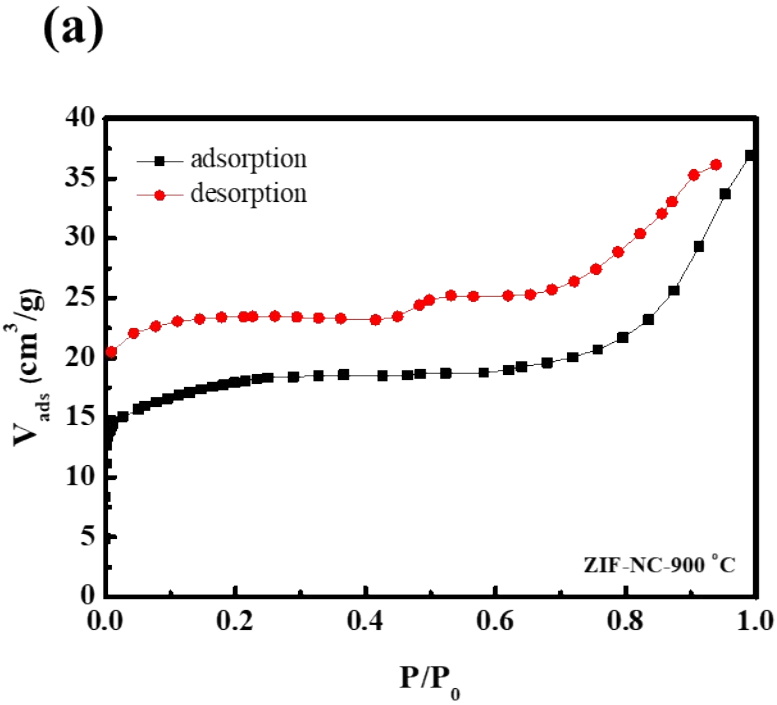
Samples[a]	η (%)	V_{OC} (V)	J_{SC} (mA cm^{-2})	FF
ZIF-ZnSe-NC-5 wt%	7.11 ± 0.04	0.76 ± 0.00	13.60 ± 0.19	0.69 ± 0.01
ZIF-ZnSe-NC-7 wt%	7.17 ± 0.07	0.79 ± 0.00	13.22 ± 0.25	0.68 ± 0.01
ZIF-ZnSe-NC-9 wt%	7.59 ± 0.17	0.79 ± 0.00	13.60 ± 0.45	0.69 ± 0.00
ZIF-ZnSe-NC-11 wt%	8.69 ± 0.13	0.77 ± 0.00	16.40 ± 0.45	0.69 ± 0.01
ZIF-ZnSe-NC-13 wt%	7.91 ± 0.05	0.75 ± 0.00	16.78 ± 0.09	0.63 ± 0.01

[a] Average values and standard deviations were obtained from three independent cells.

Table S4 The photovoltaic parameters of the DSSCs with the CEs of ZIF-ZnSe-NC-11 wt% and Pt, measured under 10-100 mW cm^{-2}.

Light intensity (mW cm^{-2})	ZIF-ZnSe-NC-11 wt%[a]			
	η (%)	V_{OC} (V)	J_{SC} (mA cm^{-2})	*FF*
100 (1 sun)	8.69 ± 0.13	0.77 ± 0.00	16.40 ± 0.45	0.69 ± 0.01
50 (0.5 sun)	8.02 ± 0.01	0.73 ± 0.00	7.60 ± 0.05	0.72 ± 0.00
10 (0.1 sun)	7.99 ± 0.01	0.68 ± 0.00	1.63 ± 0.01	0.72 ± 0.00
Light intensity (mW cm^{-2})	Pt[a]			
	η (%)	V_{OC} (V)	J_{SC} (mA cm^{-2})	*FF*
100 (1 sun)	8.26 ± 0.02	0.75 ± 0.00	16.05 ± 0.03	0.69 ± 0.00
50 (0.5 sun)	7.87 ± 0.05	0.72 ± 0.00	7.56 ± 0.03	0.73 ± 0.00
10 (0.1 sun)	7.41 ± 0.02	0.66 ± 0.00	1.67 ± 0.00	0.73 ± 0.00

[a] Average values and standard deviations were obtained from three independent cells.



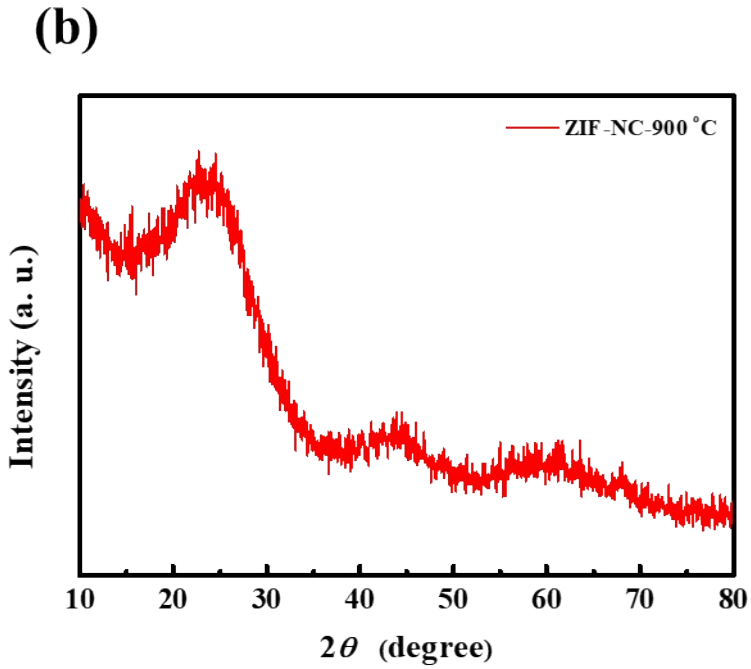
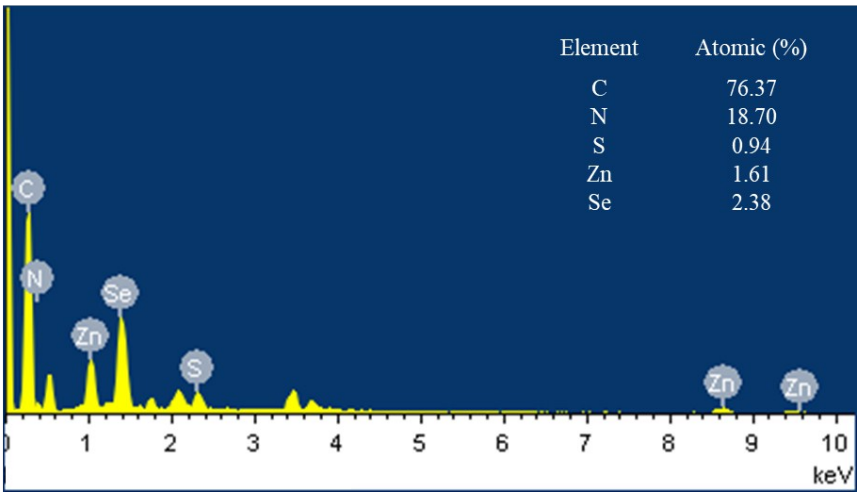


Fig. S1 (a) N_2 adsorption-desorption isotherms and (b) XRD pattern of ZIF-NC-900 °C powder.

(a)



(b)

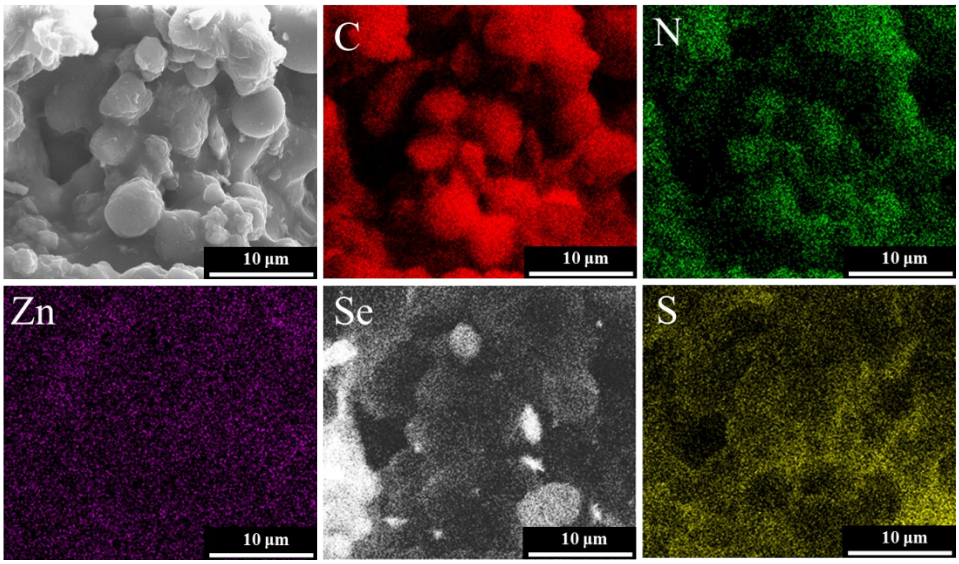


Fig. S2 (a) EDS spectrum, and (b) the corresponding EDS elemental mapping images of ZIF-ZnSe-NC-11 wt% film.

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