## **Supporting Information**

Dual-phase zinc selenide in-situ encapsulated into size-reduced ZIF-8 derived selenium and nitrogen co-doped porous carbon for efficient triiodide reduction reaction

Shuangxi Yuan,<sup>a</sup> Sining Yun,<sup>\*ab</sup> Yongwei Zhang,<sup>a</sup> Jiaoe Dang,<sup>a</sup> Menglong Sun,<sup>a</sup>

Changwei Dang,<sup>a</sup> Yingying Deng<sup>a</sup>

<sup>a</sup> Functional Materials Laboratory (FML), School of Materials Science and Engineering, Xi'an University of Architecture and Technology, Xi'an, Shaanxi, 710055, China.

<sup>b</sup> Qinghai Building and Materials Research Academy Co., Ltd, the Key Lab of Plateau Building and Eco-community in Qinghai, Xining, Qinghai, 810000, China

## \*Corresponding author

E-mail: <u>alexsyun1974@aliyun.com; yunsining@xauat.edu.cn</u>

Fax: (+86)29-82205245; Tel: (+86)29-82205245



**Figure S1.** SEM-EDS mapping image (a) with N, Zn, Se, and C elements into PS N- $C_{SR}$ . SEM images (b) and its corresponding SEM-EDS spectrum (c) for PS N- $C_{SR}$ .



Figure S2. Magnified pore distribution curves at mesoporous regions and macroporous regions for (a) N-C, (b) N-C<sub>SR</sub> and (c) PS N-C<sub>SR</sub>.



**Figure S3.** The equivalent circuits to the symmetric celsl with two arcs (a) and three arcs (b) in their EIS plots.



**Figure S4.** *J-V* plots (a) of the DSSCs using post-selenizing N- $C_{SR}$  catalysts with different selenization temperature, Tafel polarization curves (b), and EIS plots (c) of post-selenizing N- $C_{SR}$  catalysts with different selenization temperature.



Figure S5. XRD patterns of the selenide hybird catalysts derived from N- $C_{SR}$  under different post-selenization temperatures.

**Table S1.** Comparison of the elements contents of PS N- $C_{SR}$  from EDS spectrum and XPS survey spectrum.

Methods -	Quantitative analysis of elements (at. %)								
	Zn	Se	0	Ν	С				
SEM-EDS	3.62	1.50	7.46	19.49	67.94				
XPS	3.00	1.85	7.13	13.18	74.85				
TEM-EDS	3.08	1.44	14.26	11.74	69.48				

Table S2. Exact quantified analyses of PS  $\text{N-C}_{\text{SR}}$  and  $\text{N-C}_{\text{SR}}$  via ICP-OES.

Samples	Zn(wt. %)	Se(wt. %)
PS N-C <sub>SR</sub>	11.20	7.33
N-C <sub>SR</sub>	12.47	—

Table S3.	Quantitative	analysis	of N	species	into	PS	N-C <sub>SR</sub>	from	the	high-resolution	N	1s
spectrum.												

Quantitative analysis (at. %)							
Pyridinic N	Pyrrolic N	Graphitic N	NO <sub>x</sub>				
58.81	28.22	8.14	4.82				

**Table S4.** Comparison of the photovoltaic performances of the DSSCs assembled with the PS  $N-C_{SR}$  CE and the previous reported DSSCs using the Pt-free CE catalysts.

CEs	V <sub>oc</sub> (mV)	$J_{\rm sc}$ (mA cm <sup>-2</sup> )	FF	PCE (%)	References
PS N-C <sub>SR</sub>	0.77	17.00	0.65	8.48	This work
NiCo <sub>2</sub> S <sub>4</sub> QD@NCNTs	0.72	15.34	0.69	7.65	1
CoSe@NPC/CoSe@CNT	0.70	15.90	0.66	7.39	2
CoSe <sub>2</sub> /CS-2	0.69	15.88	0.69	7.56	3
CoSe@NPC/NCNTs-1	0.71	16.00	0.67	7.58	4
NiFeCoW@NC800-10-5	0.80	15.04	0.57	6.92	5
NiSe <sub>2</sub> -W	0.74	18.08	0.66	8.78	6
ZIF-ZnSe-NC-450°C	0.76	13.60	0.69	7.11	7
CoSe <sub>2</sub> @NC-CNTs	0.75	17.96	0.69	9.25	8
FeCo <sub>2</sub> S <sub>4</sub> -5h	0.72	14.2	0.72	7.35	9
ZnMoO <sub>4</sub> /3D-AWC	0.69	16.41	0.67	7.65	10

**Table S5.** Comparison of the electrochemical performances of selenide CEs with different selenization temperatures and the photovoltaic performances of the corresponding assembled DSSCs.

CEs	V <sub>oc</sub> (mV)	J <sub>sc</sub> (mA cm <sup>-2</sup> )	FF	PCE (%)	J <sub>lim</sub> (mA cm <sup>-2</sup> )	J <sub>0</sub> (mA cm <sup>-2</sup> ) <sup>a</sup>	$R_{\rm ct} (\Omega \ {\rm cm}^2)$
PS N-C <sub>SR 550</sub>	0.75	14.67	0.66	7.23	12.02	9.73	1.32
PS N-C <sub>SR</sub>	0.77	17.00	0.65	8.48	30.20	10.04	1.28
PS N-C <sub>SR 750</sub>	0.75	15.47	0.67	7.72	32.66	6.73	1.91

<sup>a</sup>: the  $J_0$  calculated from the **equation 3** in the main text.

## **References:**

- 1. P. Su, Q. Jiao, H. Li, Y. Li, X. Liu, Q. Wu, D. Shi, Y. Zhao, T. Wang and W. Wang, ACS Appl. Energy Mater., 2021, 4, 4344-4354.
- 2. T. Wang, Y. Li, H. Li, D. Shi, Q. Jiao, Y. Zhao, P. Su, W. Wang and Q. Wu, ACS Omega, 2020, 5, 26253-26261.
- 3. W. Li, P. Ma, F. Chen, R. Xu, Z. Cheng, X. Yin, Y. Lin and L. Wang, *Inorganic Chemistry Frontiers*, 2019, **6**, 2550-2557.
- 4. Y. Li, X. Liu, H. Li, D. Shi, Q. Jiao, Y. Zhao, C. Feng, X. Bai, H. Wang and Q. Wu, *J. Power Sources*, 2019, **422**, 122-130.
- 5. T. Wang, M. Xu, C. Ma, Y. Gu, W. Chen, Y. Li, J. Gong, T. Ji and W. Chen, *ACS Appl. Mater. Interfaces.*, 2021, **13**, 25010-25023.
- C. Lv, L. Sun, Q. Li, X. Wang, T. Zhang, Y. Cao, Z. Yang and L. Qi, *Electrochim. Acta*, 2020, 355, 136818.
- 7. S.-L. Jian, Y.-J. Huang, M.-H. Yeh and K.-C. Ho, J. Mater. Chem. A, 2018, 6, 5107-5118.
- 8. W. Wang, Q. Cui, D. Sun, Q. Yang, J. Xu, W. Liao, X. Zuo, H. Tang, G. Li and S. Jin, *J. Mater. Chem. C*, 2021, **9**, 7046-7056.
- 9. X. Zhang, P. Chen, F. Yang, L. Wang, J. Yin, J. Ding, F. Huang and Y. Wang, *Chem. Eng. J.*, 2021, **424**, 130419.
- 10. F. Han, S. Yun, J. Shi, Y. Zhang, Y. Si, C. Wang, N. Zafar, J. Li and X. Qiao, *Appl. Catal. B-Environ.*, 2020, **273**, 119004.