

Supplementary Information

Graphene-encapsulated selenium@polyaniline nanowires with three-dimensional hierarchical architecture for high-capacity aluminum-selenium batteries

Haiping Lei,^a Jiguo Tu,^{*b} Suqin Li,^a Zheng Huang,^b Yiwa Luo,^a Zhijing Yu,^a Shuqiang Jiao^{*a,b}

^a School of Metallurgical and Ecological Engineering, University of Science and Technology Beijing, Beijing 100083, PR China.

^b State Key Laboratory of Advanced Metallurgy, University of Science and Technology Beijing, Beijing 100083, PR China.

Corresponding authors:

*E-mail addresses: sjiao@ustb.edu.cn (S. Jiao) guo15@126.com (J. Tu).

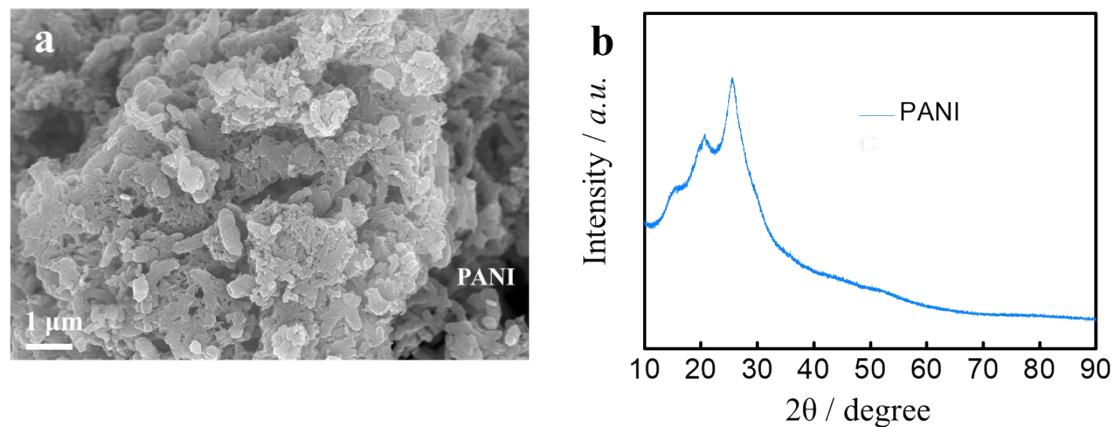


Fig. S1 (a) SEM image of PANI. (b) XRD pattern of PANI.

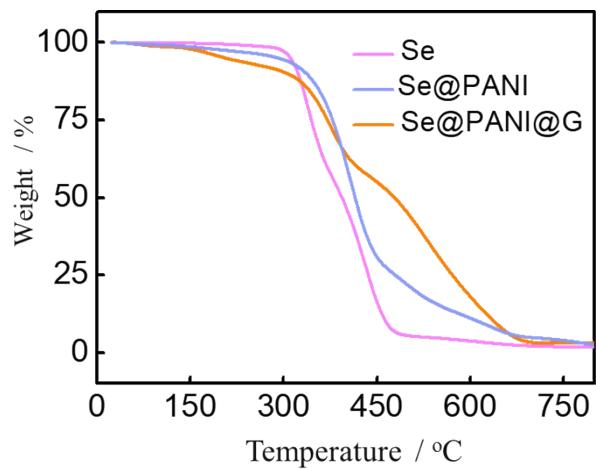


Fig. S2 TG curves of the as-prepared Se nanowires, Se@PANI, and Se@PANI@G.

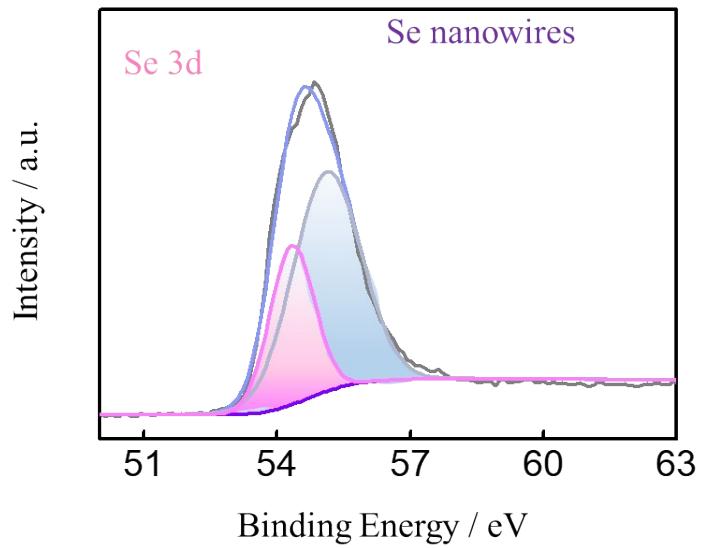


Fig. S3 Se 3d XPS spectra of as-prepared Se nanowires.

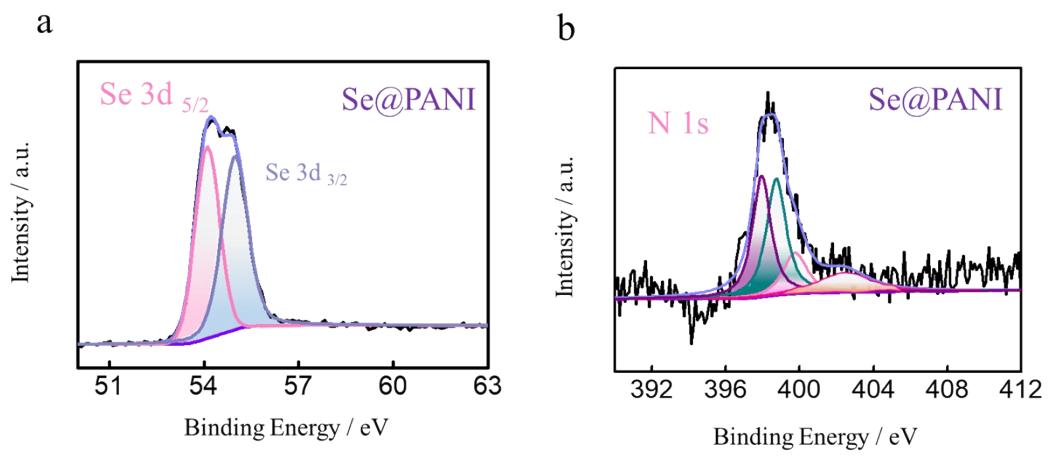


Fig. S4 (a) Se 3d XPS spectra of as-prepared Se@PANI. (b) N 1s XPS spectra of as-prepared Se@PANI.

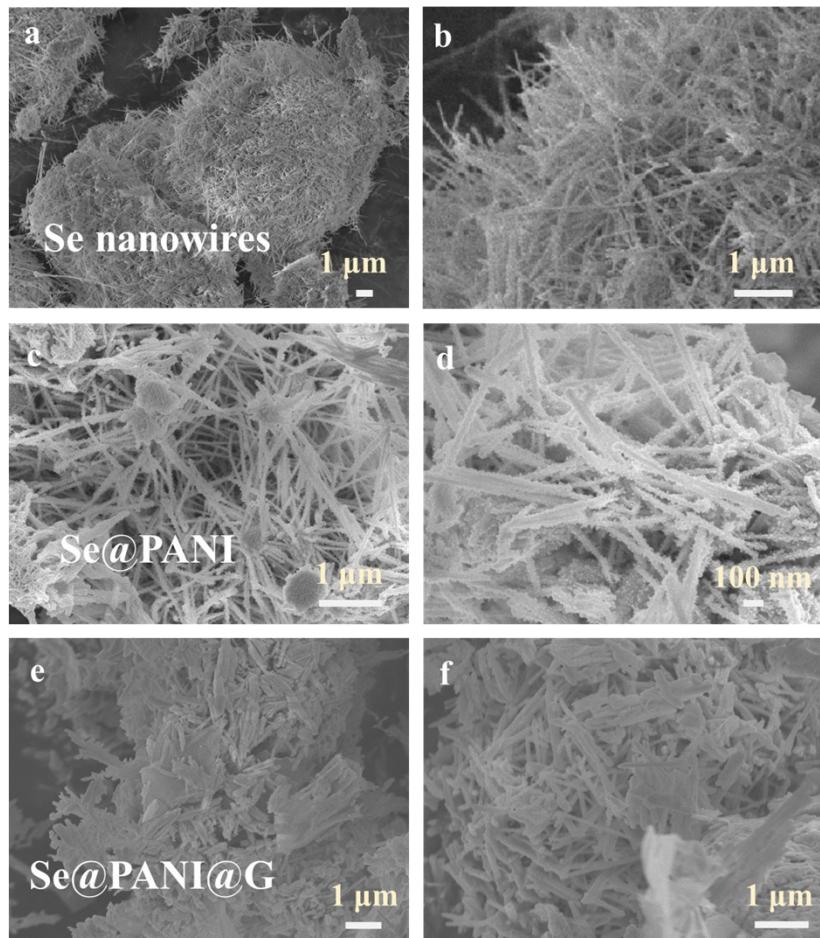


Fig. S5 (a,b) SEM images of as-prepared Se nanowires. (c,d) SEM images of as-prepared Se@PANI. (e,f) SEM images of as-prepared Se@PANI@G.

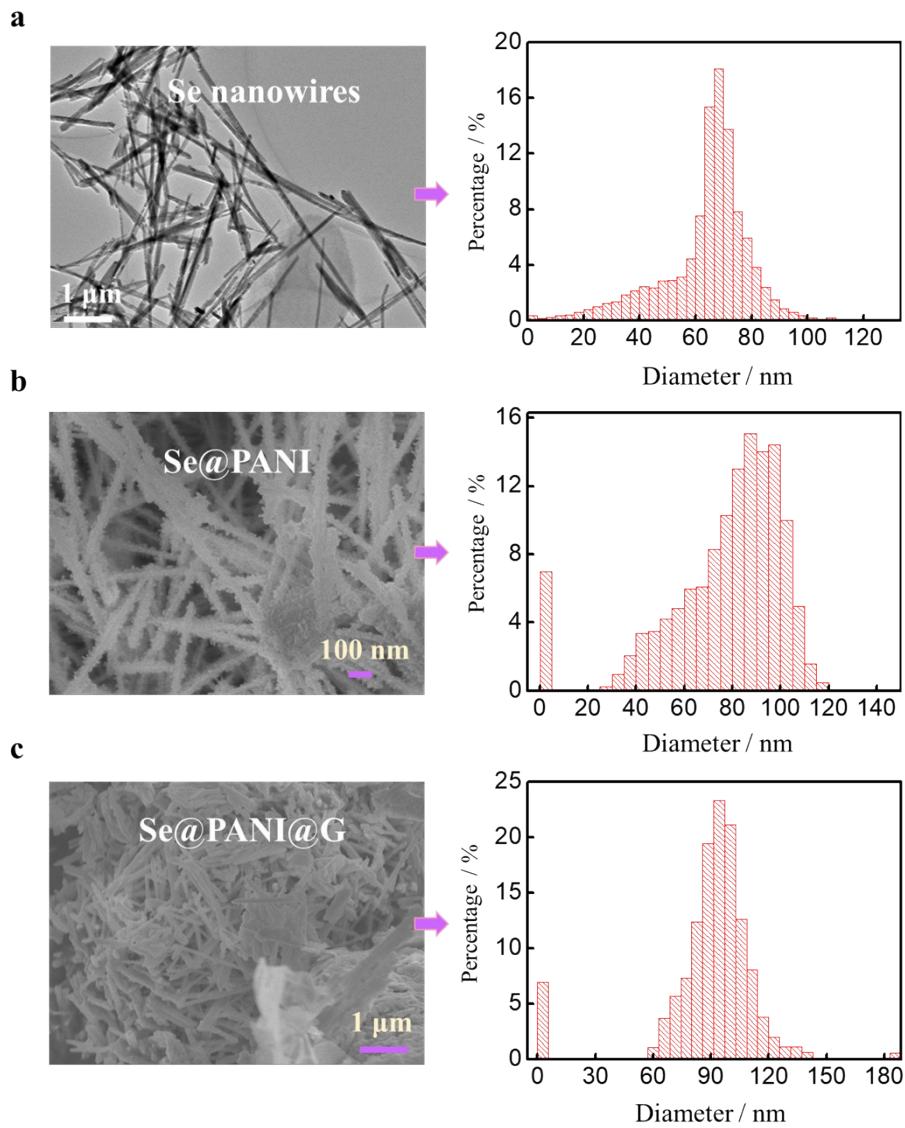


Fig. S6 (a) SEM images of as-prepared Se nanowires and the corresponding histogram of Se nanowires diameter. (b) SEM images of as-prepared Se@PANI and the corresponding histogram of Se@PANI diameter. (c) SEM images of as-prepared Se@PANI@G and the corresponding histogram of Se@PANI@G diameter.

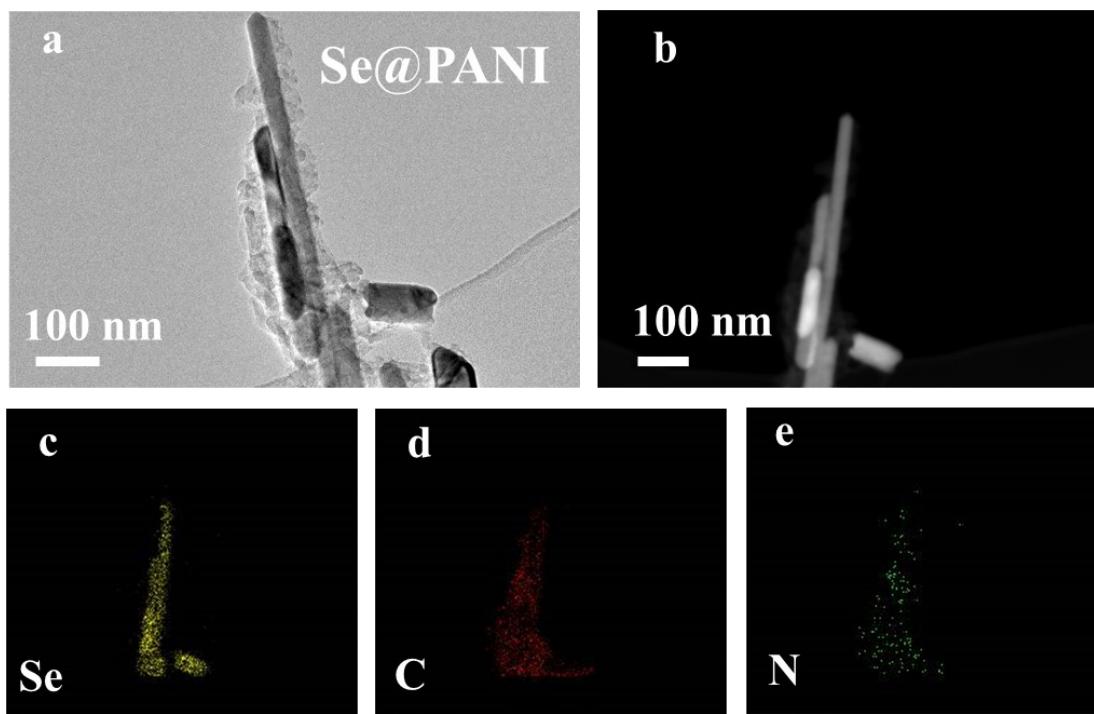


Fig. S7 (a) TEM images of Se@PANI. (b) HAADF (High-Angle Annular Dark Field)-STEM image of the Se@PANI nanowires. (c-e) The corresponding elemental mapping images.

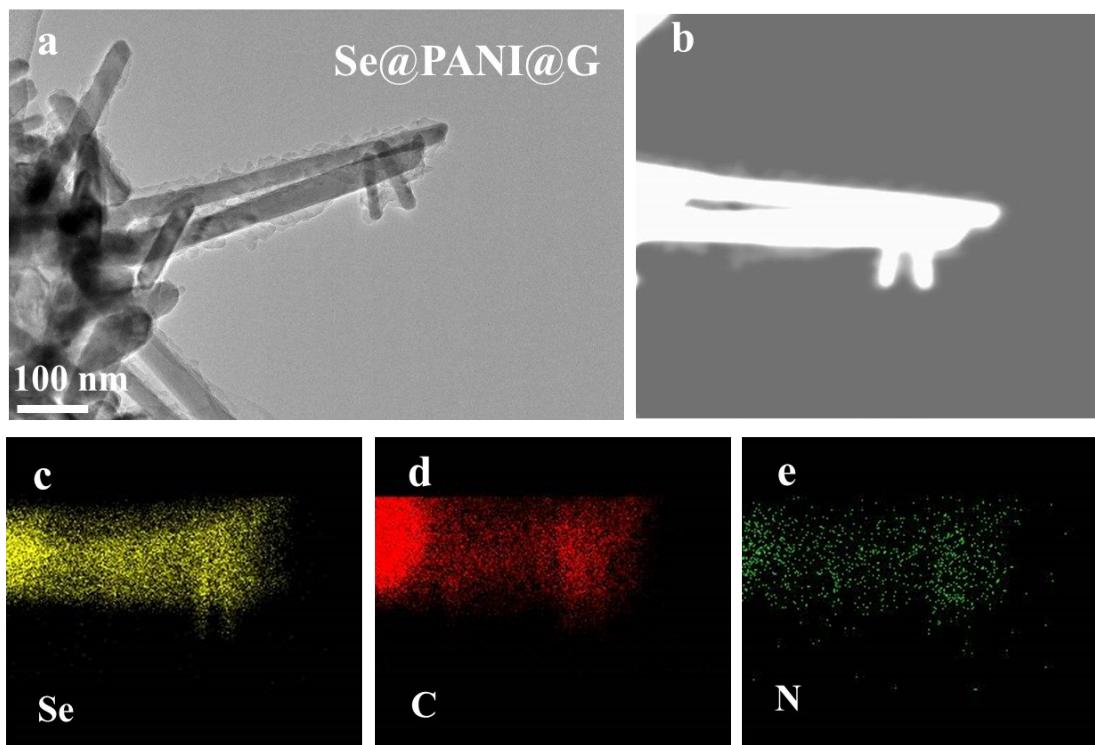


Fig. S8 (a) TEM images of Se@PANI@G. (b) HAADF-STEM image of the Se@PANI@G nanowires. (c-e) The corresponding elemental mapping images.

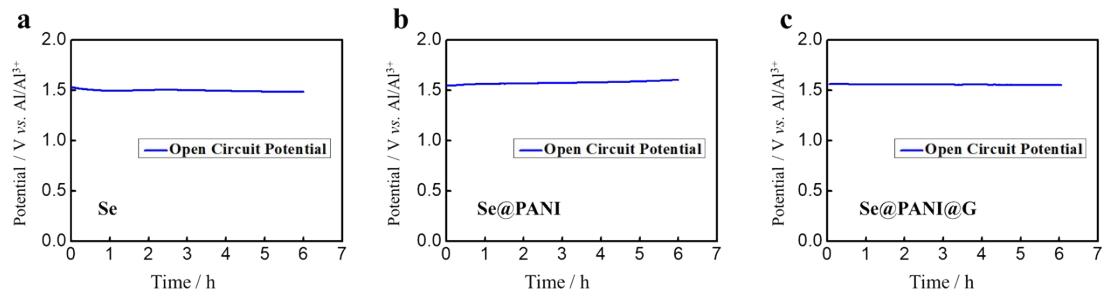


Fig. S9 (a) The open circuit potential of Al/Se battery before cycling. (b) The open potential of Al/Se@PANI battery before cycling. (c) The open potential of Al/Se@PANI@G battery before cycling.

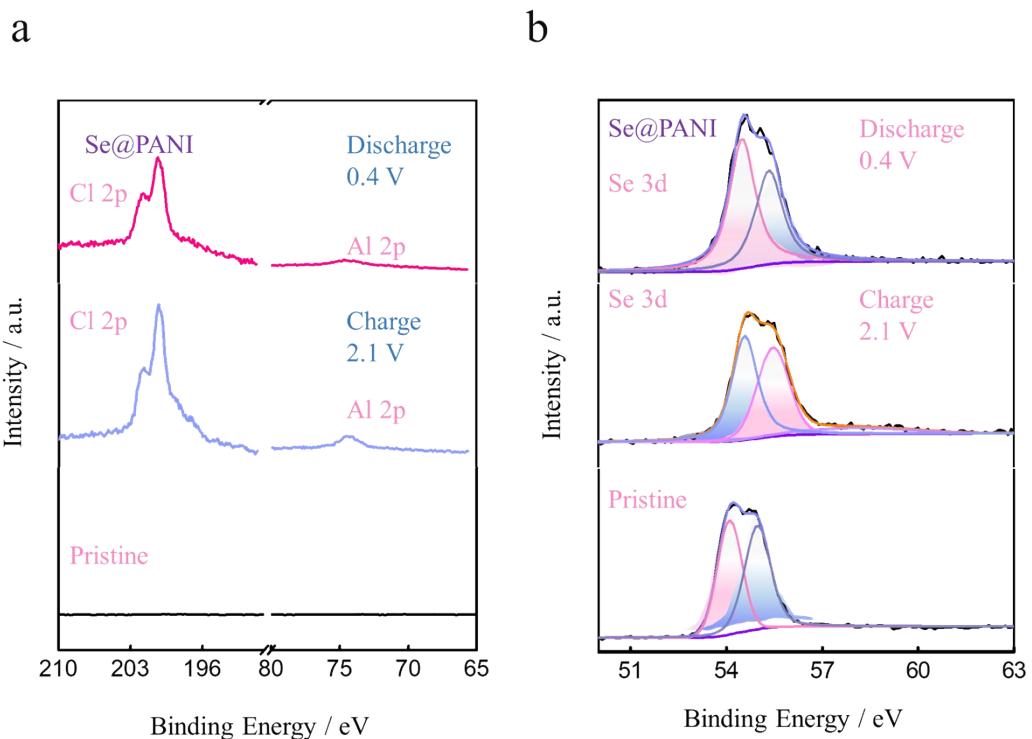
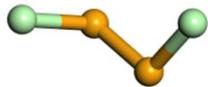


Fig. S10 (a) Al 2p, Cl 2p, and (b) Se 3d, XPS spectra of Se@PANI electrodes after charging

to 2.1 V and discharging to 0.4 V.



PANI

Top view

Side view

Fig. S11 The structures of Se_2Cl_2 and PANI.

PANI@G

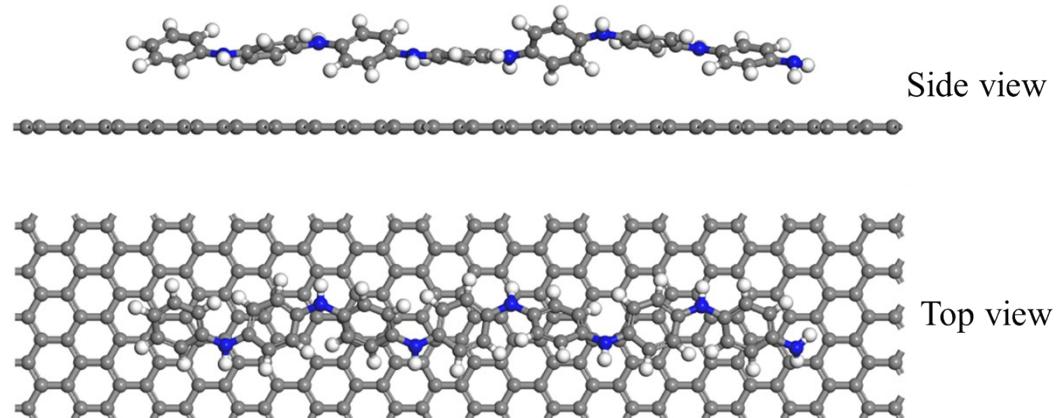


Fig. S12 The optimized structures of PANI@G.

Table S1 The total energies of Se_2Cl_2 , PANI, PANI@G, PANI@ Se_2Cl_2 , and PANI@G@ Se_2Cl_2 .

	Total energy/eV
Se_2Cl_2	-155720.4302
PANI	-54531.86008
PANI@G	-236923.1305
PANI@ Se_2Cl_2	-210254.4815
PANI@G@ Se_2Cl_2	-392647.2731

Table S2 Comparison of electrochemical performances of Se@PANI@G positive electrode with previous Se-based positive electrodes.

Positive electrode	Electrolyte	Separator	Voltage range (V)	Discharge capacity (mAh g ⁻¹)	Current density (mA g ⁻¹)	Cycles
Se/graphene aerogel (Se/GA) ^[1]	AlCl ₃ /Et ₃ NHCl, 1.5:1 by mole	glass fiber(GF/D) oxidizing CNT (O-CNT) modified separator	0.01-2.3	~176	1000	50
Se/GA ^[1]	AlCl ₃ /Et ₃ NHCl, 1.5:1 by mole	glass fiber(GF/C)	0.01-2.3	395	1000	200
MCF-7/Se ^[2]	EMImCl/AlCl ₃ , 1: 1.1 by mole		1.0-2.3	152	500	2000
TiO ₂ @Se-rGO ^[3]	EMImCl/AlCl ₃ , 1: 1.3 by mole	Whatman glass fiber (GF/C)	0.1-2.2	225.8	500	500
Se ^[4]	EMImCl/AlCl ₃ , 1: 1.3 by mole	CMK-3 modified separators	0.01-2.4	270	1000	500
Se nanowires grown directly on a flexible carbon cloth substrate (Se NWs@CC) [5]	Thiourea-AlCl ₃		0.01-1.5	195	100	100
Se@CMK-3 ^[6]	EMImCl/AlCl ₃ , 1: 1.3 by mole	Whatman GF/D	0.05-1.5	600	67.5	9
one-dimensional hollow Se@C nanotube (Se@CT) ^[7]	EMImCl/AlCl ₃ , 1: 1.3 by mole	Whatman glass fiber (GF/C)	0.5-2.3	162.9	500	200
Se nanowires and mesoporous carbon (Se/CMK-3) ^[8]	EMImCl-AlCl ₃ , 1:1.1 by mole	Glass fiber (Filtech)	1.0-2.3	124	200	50
This work (Se@PANI@G)	EMImCl/AlCl ₃ , 1: 1.3 by mole	glass fiber (GF/A)	0.4-2.1	164	200	160

References

- 1 T. Zhang, T. Cai, W. Xing, T. Li, B. Liang, H. Hu, L. Zhao, X. Li and Z. Yan, *Energy Storage Mater.*, 2021, **41**, 667-676.
- 2 Y. Kong, A. K. Nanjundan, Y. Liu, H. Song, X. Huang and C. Yu, *Small*, 2019, **15**, 1904310.
- 3 Z. Li, X. Wang, X. Li and W. Zhang, *Chem. Eng. J.*, 2020, **400**, 126000.
- 4 H. Lei, S. Jiao, J. Tu, W. L. Song, X. Zhang, M. Wang, S. Li, H. Chen and D. Fang, *Chem. Eng. J.*, 2020, **385**, 123452.
- 5 S. C. Wu, Y. Ai, Y. Z.Chen, K. Wang, T. Y. Yang, H. J. Liao, T. Y. Su, S. Y.Tang, C. W. Chen, D. C. Wu, Y. C. Wang, A. Manikandan, Y. C. Shih, L. Lee and Y. L. Chueh, *ACS Appl. Mater. Interfaces*, 2020, **12**, 27064-27073.
- 6 S. Liu, X. Zhang, S. He, Y. Tang, J. Wang, B. Wang, S. Zhao, H. Su, Y. Ren, L. Zhang, J. Huang, H. Yu, K. Amine, *Nano Energy*, 2019, **66**, 104159.
- 7 Z. Li, J. Liu, X. Huo, J. Li and F. Kang, *ACS Appl. Mater. Interfaces*, 2019, **11**, 45709-45716.
- 8 X. Huang, Y. Liu, C. Liu, J. Zhang, O. Nooan and C. Yu, *Chem. Sci.*, 2018, **9**, 5178-5182.