Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary Information

$MoSe_2$/N-Doped Hollow Carbon Spheres Host for Rechargeable Na-Se batteries

Fengping Xiao‡[a,b], Peng Hu‡[a,b*], Yanni Wu[a,d], Qing Tang[a], Nilesh Shinde[b], Yulong Liu[c]

[a] *School of Environment and Chemical Engineering, Zhaoqing University, Zhaoqing, Guangdong 526061, P. R. China*

[b] *Department of Chemistry, The University of Western Ontario, London, Ontario N6A 5B7, Canada*

[c] *Department of Chemistry, Northeast Normal University, 5268 Renming Street, Changchun, China*

[d] *Guangdong Provincial Key Laboratory of Environmental Health and Land Resource, Zhaoqing University, Zhaoqing, Guangdong 526061, P. R. China*

Table S1. Summary comparison of cyclic performances of Na-Se batteries, the specific capacity was calculated based on Se content.

Material	Current density [mA g^{-1}]	Cyclability [mAh g_{se}^{-1}] (after cycles)	Selenium content [wt%]	Year/Ref
N-doped porous carbon hollow spheres@$MoSe_2$	**1000**	**493 (1000)**	**72**	**This work**
Se@hollow mesoporous carbon sphere	500	291 (1500)	56	2020/[1]
N, S-co-doped hierarchically porous carbon microspheres/Se	338	445 (400)	59	2020/[2]
Jackfruit-like Se-carbon	1350	392 (600)	53	2019/[3]
Se/S, O co-doped hierarchical porous carbon	338	265 (600)	50	2019/[4]
Se@N-doped interconnected carbon aerogels	500	407 (800)	52	2019/[5]
Se impregnated carbonized leaf	2000	300 (500)	47	2019/[6]
PANI@N, S dual-doped hierarchical porous carbon/Se	1350	480 (1000)	57	2019/[7]
Se@microporous carbon nanofibers	500	430 (300)	48	2018/[8]
Se-hierarchical porous carbon	1350	243 (1000)	56	2018/[9]
Se/N-doped microporous carbon polyhedrons	1000	460 (500)	49	2018/[10]
Se@N-doped hierarchically radial-structured carbon	338	~ 400 (500)	62	2018/[11]

Se/N, O dual-doped hierarchical porous carbon	338	402 (500)	48	2018/[12]
Al_2O_3 coated (Se/porous N-doped carbon nanofibers)@Se	500	503 (1000)	67	2018/[13]
Se-monolithic carbon	135	~ 400 (150)	70	2018/[14]
Carbon nanofiber/Se	67.5	374 (94)	72	2018/[15]
Se@N, O dual-doped porous carbon sheet-CNT film	1000	400 (2000)	60	2018/[16]
Se/N-doped porous carbon polyhedrons	1350	161 (1000)	49	2017/[17]
Se-carbon nanosheet	135	514 (500)	53	2017/[18]
Se@mesoporous carbon nanofibers	50	520 (80)	52	2015/[19]
Se@carbon nanofiber-CNT	500	410 (240)	35	2015/[20]
in-situ formed C/Se composite	100	280(50)	54	2015/[21]
Se@mesoporous carbon composite	67.5	340 (380)	30	2013/[22]

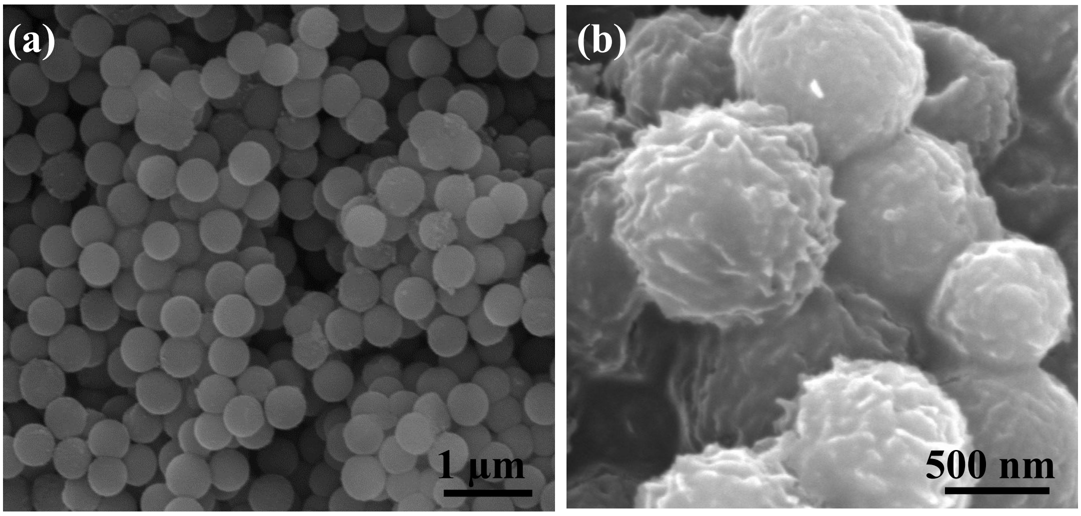

Figure S1. SEM image of (a) SiO_2 spheres and (b) SiO_2@$MoSe_2$/N-doped carbon composite.

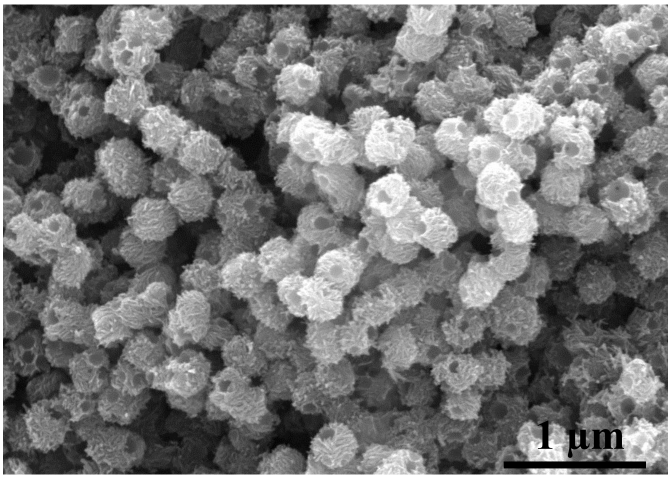

Figure S2. SEM image of the NCHS@$MoSe_2$ host.

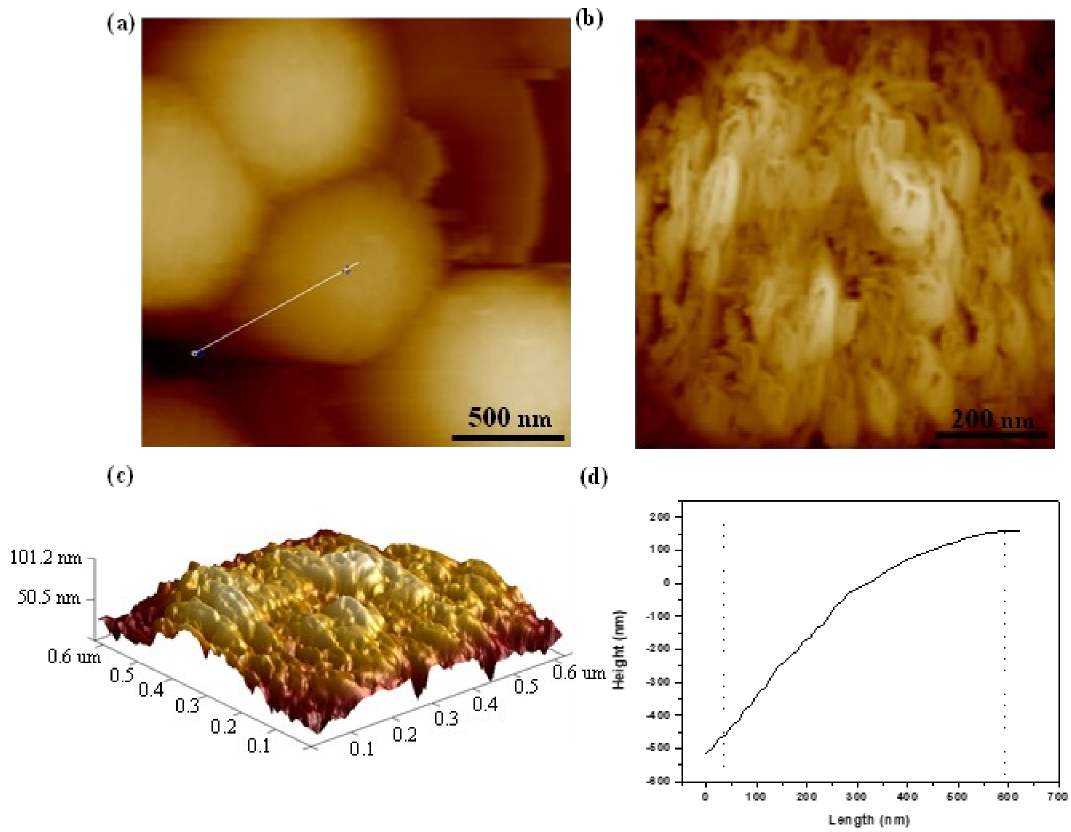

Figure S3. Tapping-mode AFM images of the topography of NCHS@$MoSe_2$ under (a) low and (b) high resolutions, (c) the corresponding 3D view, and (d) the corresponding line scan.

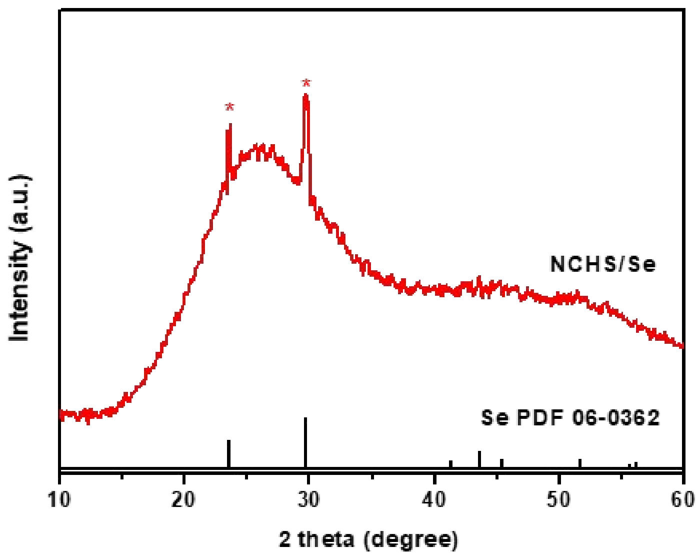

Figure S4. XRD pattern of the NCHS/Se composite (Se peaks are marked with red asterisks).

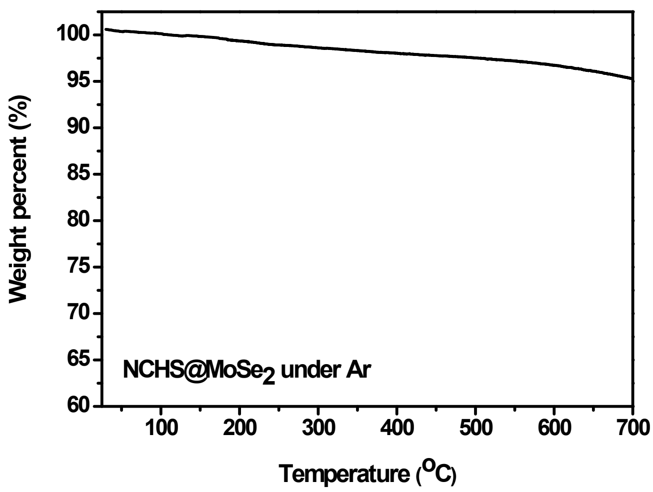

Figure S5. TGA curve of the NCHS@$MoSe_2$ composite under Ar.

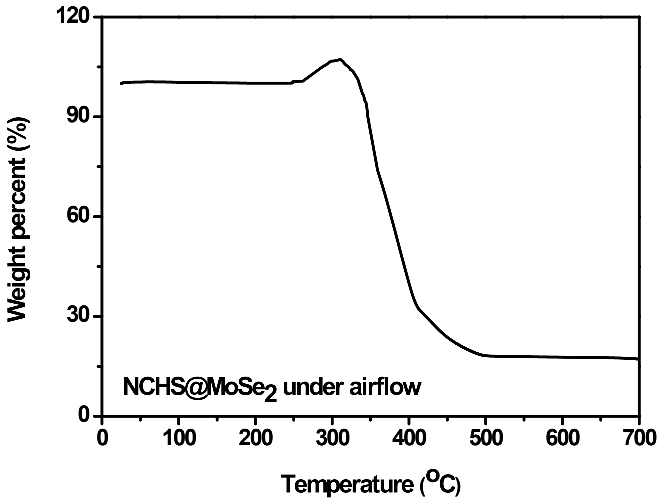

Figure S6. TGA curve of NCHS@$MoSe_2$ composite under airflow.

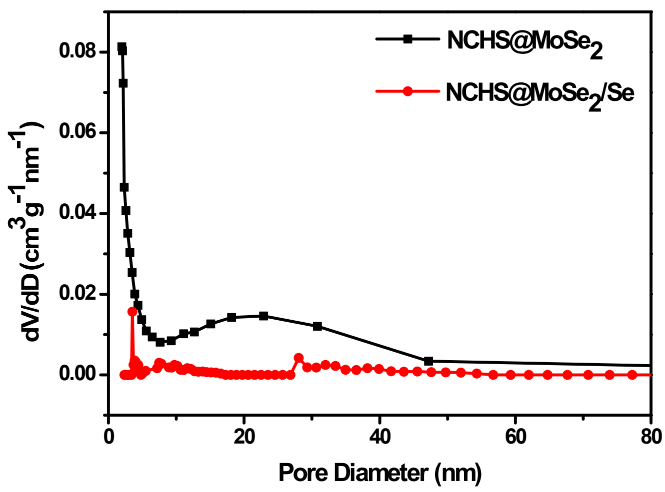

Figure S7. The pore size distribution of NCHS@$MoSe_2$ and NCHS@$MoSe_2$/Se composites.

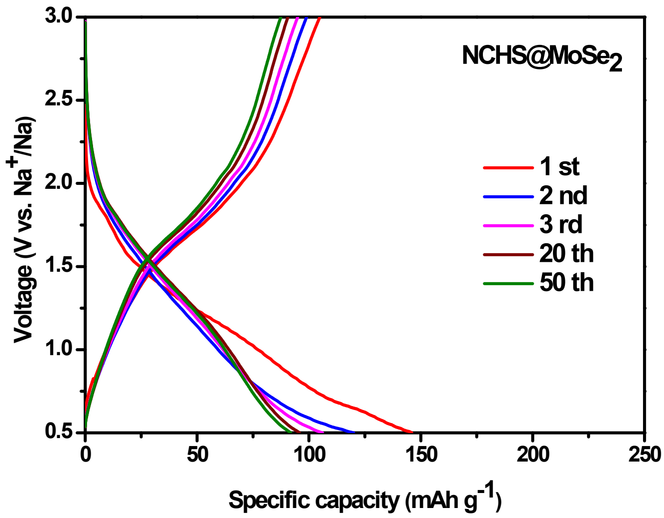

Figure S8. The cycle performance of NCHS@$MoSe_2$ electrode at 0.1 A g^{-1}.

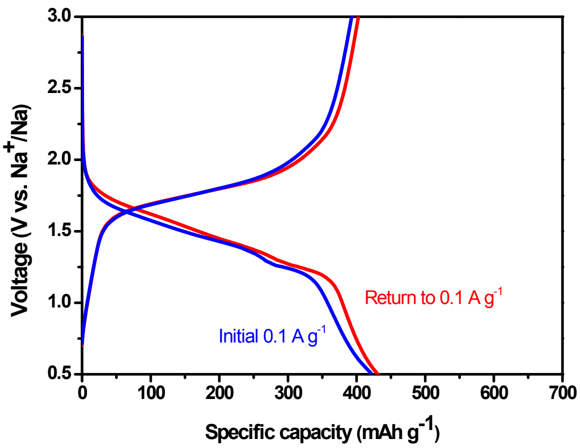

Figure S9. Selected charge/discharge profiles of NCHS@$MoSe_2$/Se cathode at the initial and return to 0.1 A g^{-1}.

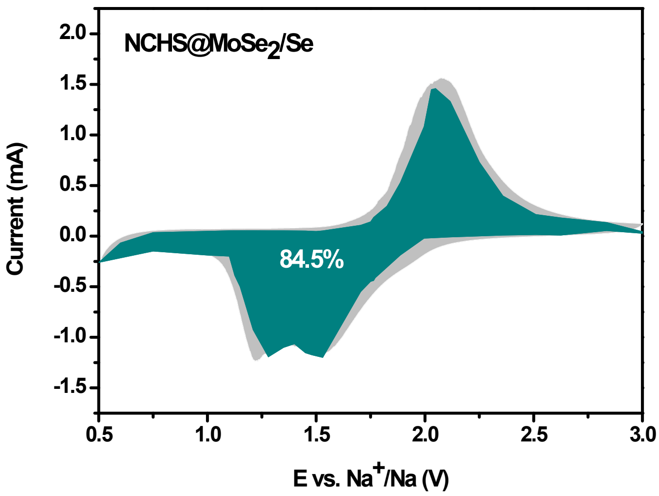

Figure S10. The illustration of the pseudocapacitive fraction at 1.0 mVs^{-1}.

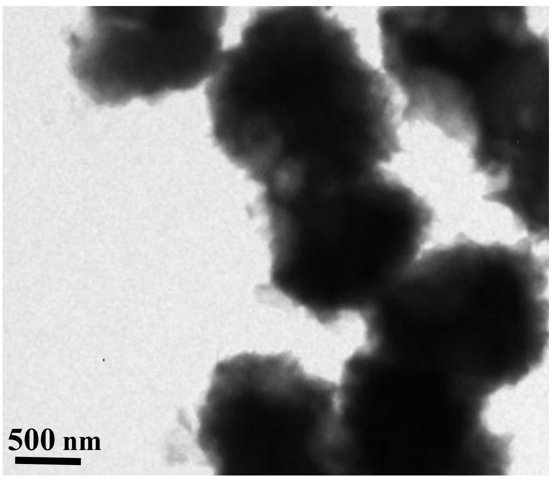

Figure S11. TEM image of NCHS@$MoSe_2$/Se cathode after 100 cycles.

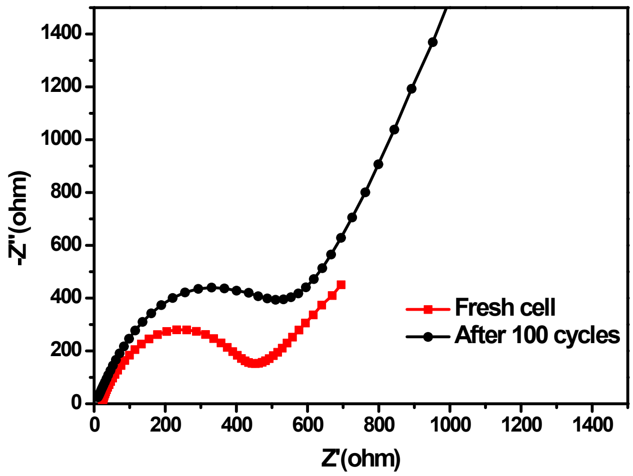

Figure S12. EIS characterization of NCHS@$MoSe_2$/Se before and after 100 cycles.

References

[1] Xue, P.; Zhai, Y.; Wang, N.; Zhang, Y.; Lu, Z.; Liu, Y.; Bai, Z.; Han, B.; Zou, G.; Dou, S. Selenium@Hollow Mesoporous Carbon Composites for High-Rate and Long-Cycling Lithium/Sodium-Ion Batteries. *Chem. Eng. J.* **2020,** *392*, 123676.

[2] Kim J. K. Kang Y. C. Encapsulation of Se into Hierarchically Porous Carbon Microspheres with Optimized Pore Structure for Advanced Na−Se and K−Se Batteries. *ACS Nano* **2020**, *14*, 13203−13216

[3] Xu, Q.; Yang, T.; Gao, W.; Zhan, R.; Zhang, Y.; Bao, S.; Li, X.; Chen, Y.; Xu, M. Jackfruit-Like Electrode Design for Advanced Na-Se Batteries. *J. Power Sources* **2019,** *443*, 227245.

[4] Zhao, X.; Yin, L.; Yang, Z.; Chen, G.; Yue, H.; Zhang, D.; Sun, Z.; Li, F. An Alkali Metal-Selenium Battery with a Wide Temperature Range and Low Self-Discharge. *J. Mater. Chem. A* **2019,** *7*, 21774-21782.

[5] Deng, Y.; Gong, L.; Pan, Y.; Cheng, X.; Zhang, H. A Long-Life Sodium–Selenium Cathode by Encapsulating Selenium into N-Doped Interconnected Carbon Aerogels. *Nanoscale* **2019,** *11*, 11671-11678.

[6] Guo, B.; Mi, H.; Zhang, P.; Ren, X.; Li, Y. Free-Standing Selenium Impregnated Carbonized Leaf Cathodes for High-Performance Sodium-Selenium Batteries. *Nanoscale Res. Lett.* **2019,** *14*, 30.

[7] Zhang, F.; Xiong, P.; Guo, X.; Zhang, J.; Yang, W.; Wu, W.; Liu, H.; Wang, G. A Nitrogen, Sulphur Dual-Doped Hierarchical Porous Carbon with Interconnected Conductive Polyaniline Coating for High-Performance Sodium-Selenium Batteries. *Energy Storage Mater.* **2019,** *19*, 251-260.

[8] Yuan, B.; Sun, X.; Zeng, L.; Yu, Y.; Wang, Q. A Freestanding and Long-Life Sodium-Selenium Cathode by Encapsulation of Selenium into Microporous Multichannel Carbon Nanofibers. *Small* **2018,** *14*, 1703252.

[9] Xu, Q.; Liu, H.; Du, W.; Zhan, R.; Hu, L.; Bao, S.; Dai, C.; Liu, F.; Xu, M. Metal-Organic Complex Derived Hierarchical Porous Carbon as Host Matrix for Rechargeable Na- Se Batteries. *Electrochim. Acta* **2018,** *276*, 21-27.

[10] Li, S.; Yang, H.; Xu, R.; Jiang, Y.; Gong, Y.; Gu, L.; Yu, Y. Selenium Embedded in MOF-Derived N-Doped Microporous Carbon Polyhedrons as a High Performance Cathode for Sodium-Selenium Batteries. *Mater. Chem. Front.* **2018,** *2*, 1574-1582.

[11] Dong, W.; Chen, H.; Xia, F.; Yu, W.; Song, J.; Wu, S.; Deng, Z.; Hu, Z.-Y.; Hasan, T.; Li, Y.; Wang, H.; Chen, L.; Su, B.-L. Selenium Clusters in Zn-Glutamate MOF Derived Nitrogen-Doped Hierarchically Radial-Structured Microporous Carbon for Advanced Rechargeable Na-Se Batteries. *J. Mater. Chem. A* **2018,** *6*, 22790-22797.

[12] Zhao, X.; Yin, L.; Zhang, T.; Zhang, M.; Fang, Z.; Wang, C.; Wei, Y.; Chen, G.; Zhang, D.; Sun, Z.; Li, F. Heteroatoms Dual-Doped Hierarchical Porous Carbon-Selenium Composite for Durable Li-Se and Na-Se Batteries. *Nano Energy* **2018,** *49*, 137-146.

[13] Ma, D.; Li, Y.; Yang, J.; Mi, H.; Luo, S.; Deng, L.; Yan, C.; Zhang, P.; Lin, Z.; Ren, X.; Li, J.; Zhang, H. Atomic Layer Deposition-Enabled Ultrastable Freestanding Carbon- Selenium Cathodes with High Mass Loading for Sodium-Selenium Battery.

Nano Energy **2018,** *43*, 317-325.
[14] Ding, J.; Zhou, H.; Zhang, H.; Tong, L.; Mitlin, D. Selenium Impregnated Monolithic Carbons as Free-Standing Cathodes for High Volumetric Energy Lithium and Sodium Metal Batteries. *Adv. Energy Mater.* **2018,** *8*, 1701918.
[15] Wang, H.; Jiang, Y.; Manthiram, A. Long Cycle Life, Low Self-Discharge Sodium- Selenium Batteries with High Selenium Loading and Suppressed Polyselenide Shuttling. *Adv. Energy Mater.* **2018,** *8*, 1701953.
[16] Yao, Y.; Chen, M.; Xu, R.; Zeng, S.; Yang, H.; Ye, S.; Liu, F.; Wu, X.; Yu, Y. CNT Interwoven Nitrogen and Oxygen Dual-Doped Porous Carbon Nanosheets as Free-Standing Electrodes for High-Performance Na-Se and K-Se Flexible Batteries. *Adv. Mater.* **2018,** *30*, 1805234.
[17] Xu, Q.; Liu, T.; Li, Y.; Hu, L.; Dai, C.; Zhang, Y.; Li, Y.; Liu, D.; Xu, M. Selenium Encapsulated into Metal-Organic Frameworks Derived N-Doped Porous Carbon Polyhedrons as Cathode for Na-Se Batteries. *ACS Appl. Mater. Interfaces* **2017,** *9*, 41339-41346.
[18] Ding, J.; Zhou, H.; Zhang, H.; Stephenson, T.; Li, Z.; Karpuzov, D.; Mitlin, D. Exceptional Energy and New Insight with a Sodium-Selenium Battery Based on a Carbon Nanosheet Cathode and a Pseudographite Anode. *Energy Environ. Sci.* **2017,** *10*, 153-165.
[19] Zeng, L.; Zeng, W.; Jiang, Y.; Wei, X.; Li, W.; Yang, C.; Zhu, Y.; Yu, Y. A Flexible Porous Carbon Nanofibers-Selenium Cathode with Superior Electrochemical Performance for Both Li-Se and Na-Se Batteries. *Adv. Energy Mater.* **2015,** *5*, 1401377.
[20] Zeng, L.; Wei, X.; Wang, J.; Jiang, Y.; Li, W.; Yu, Y. Flexible One-Dimensional Carbon-Selenium Composite Nanofibers with Superior Electrochemical Performance for Li- Se/Na-Se Batteries. *J. Power Sources* **2015,** *281*, 461-469.
[21] Luo, C.; Wang, J.; Suo, L.; Mao, J.; Fan, X.; Wang, C. *in Situ* Formed Carbon Bonded and Encapsulated Selenium Composites for Li-Se and Na-Se Batteries. *J. Mater. Chem. A* **2015,** *3*, 555-561.
[22] Luo, C.; Xu, Y.; Zhu, Y.; Liu, Y.; Zheng, S.; Liu, Y.; Langrock, A.; Wang, C. Selenium@Mesoporous Carbon Composite with Superior Lithium and Sodium Storage Capacity. *ACS Nano* **2013,** *7*, 8003-801