

**Anchoring intermediate phases via few-layer MoS<sub>2</sub> nanosheets in flexible porous carbon fiber for stable lithium ion storage**

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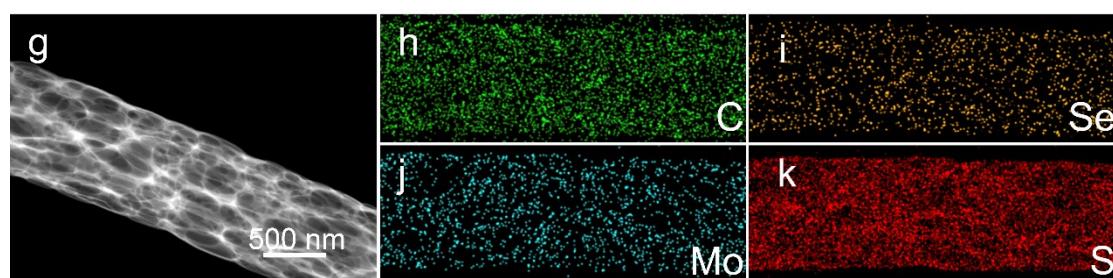
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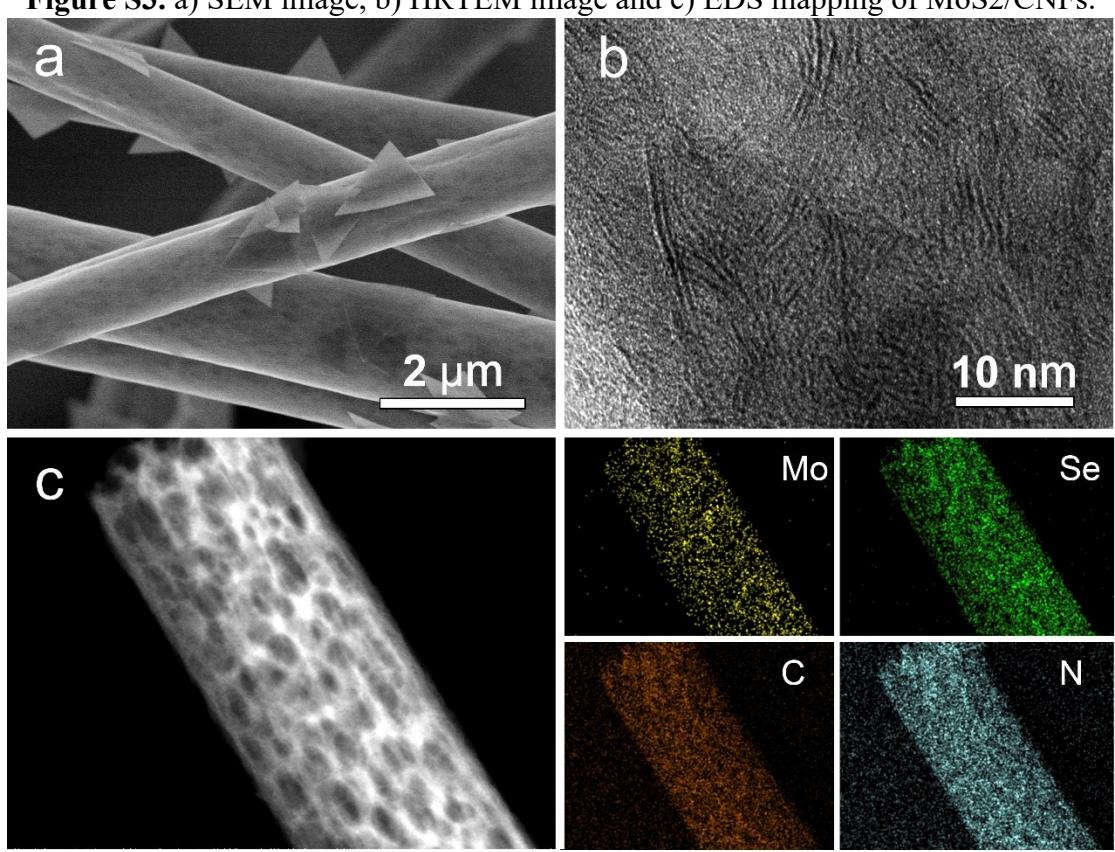
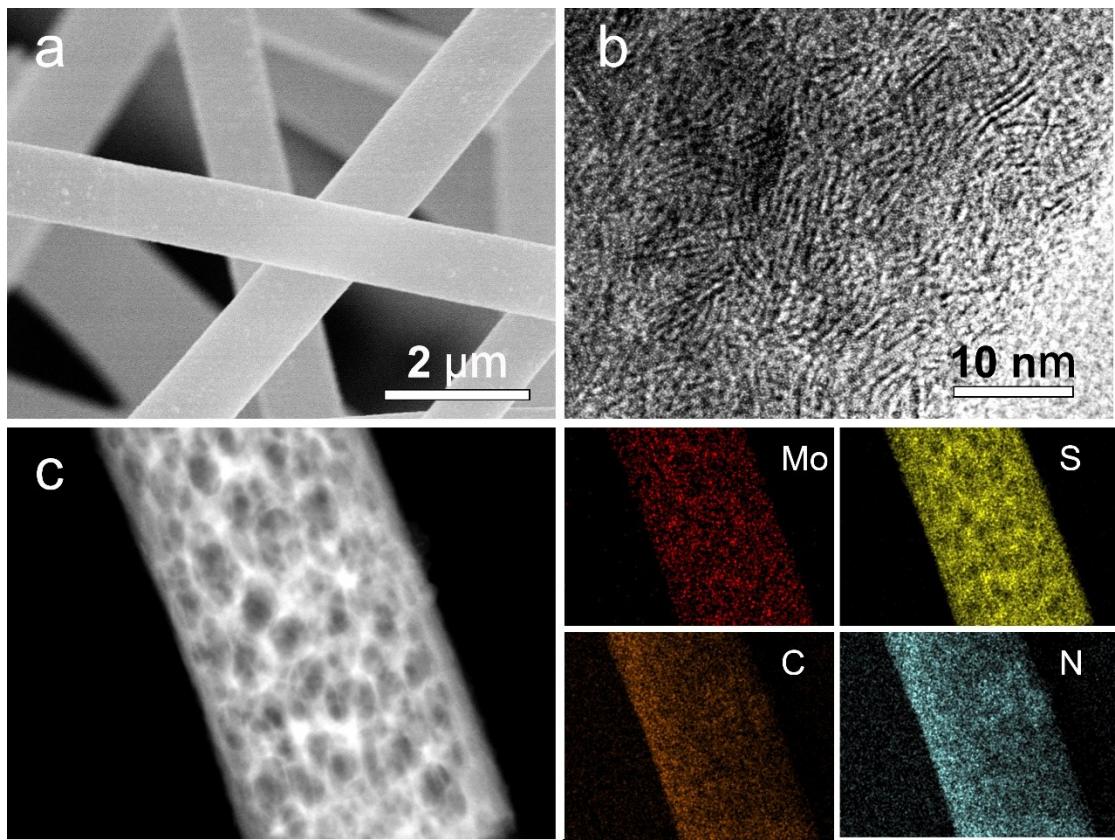
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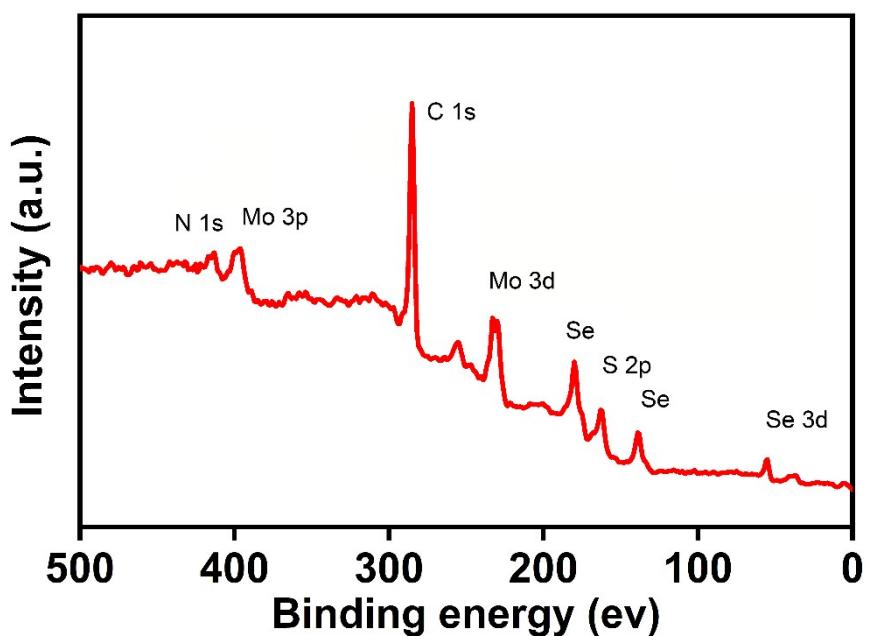


**Figure S1.** Optical photographs of MoS<sub>2</sub>/CNFs film.

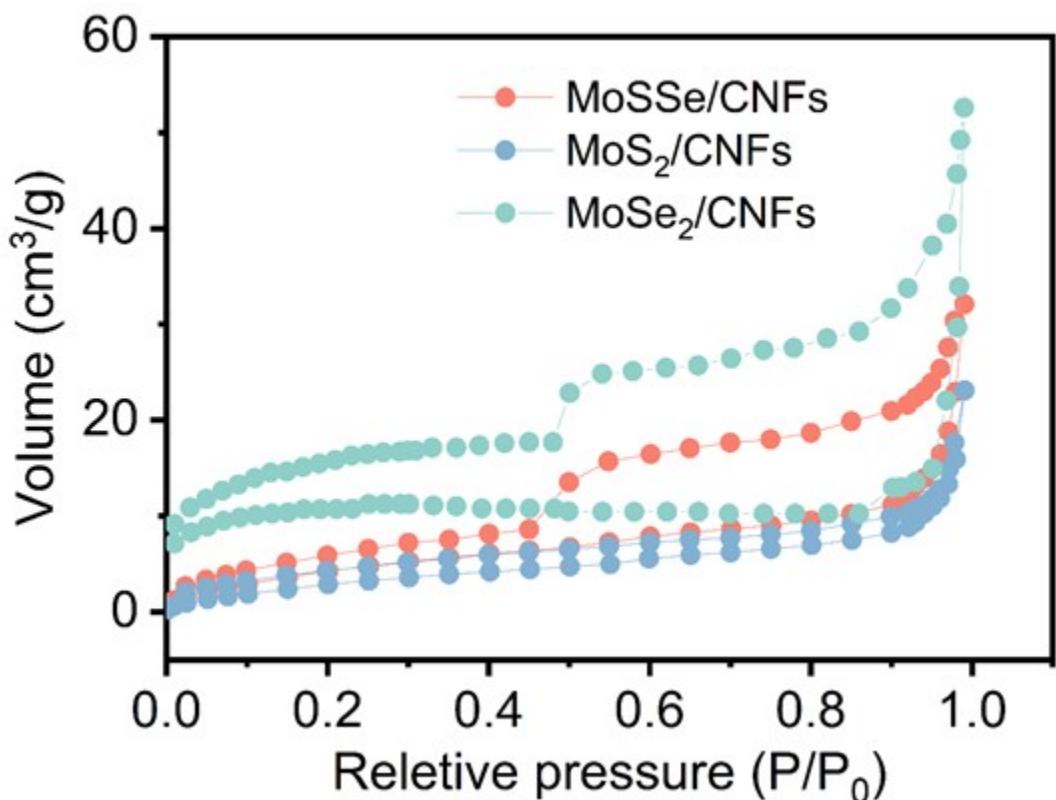


**Figure S2.** EDS mapping of MoS<sub>2</sub>/CNFs.

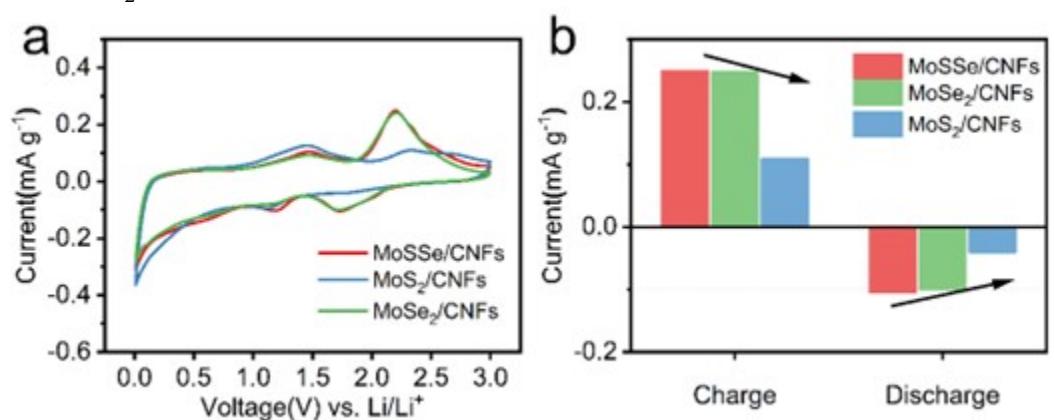
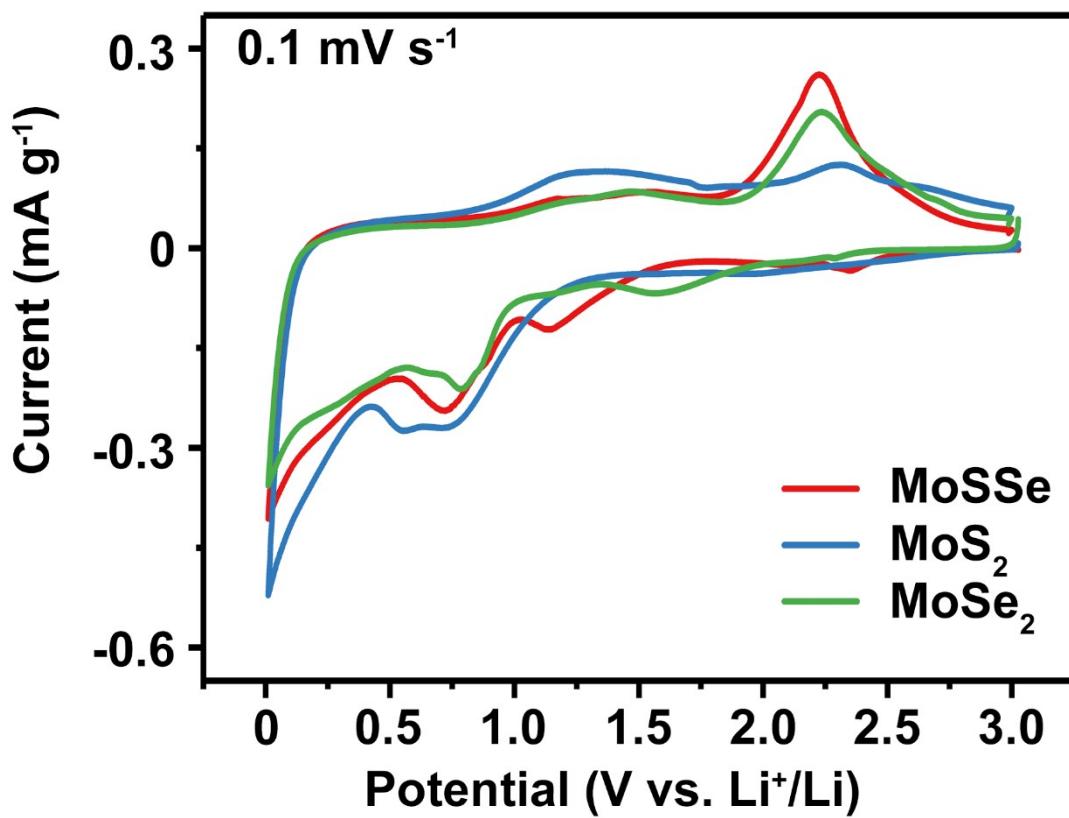




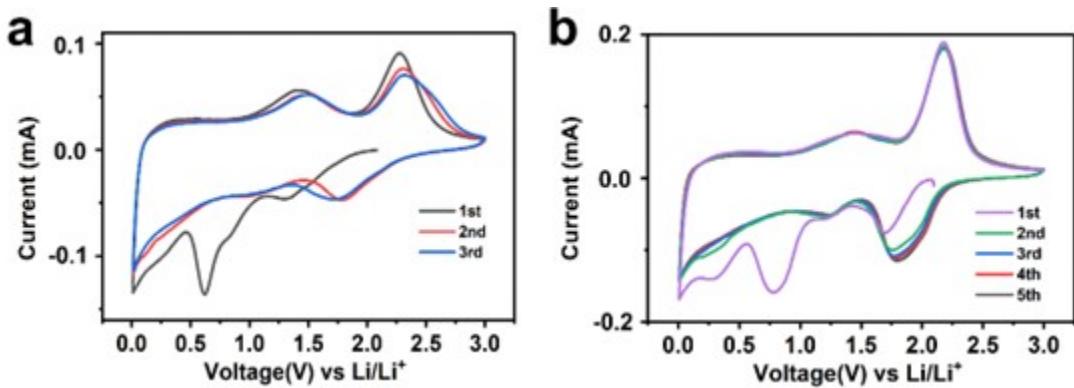
**Figure S5.** The XPS survery spectrum of MoSSe/CNFs.



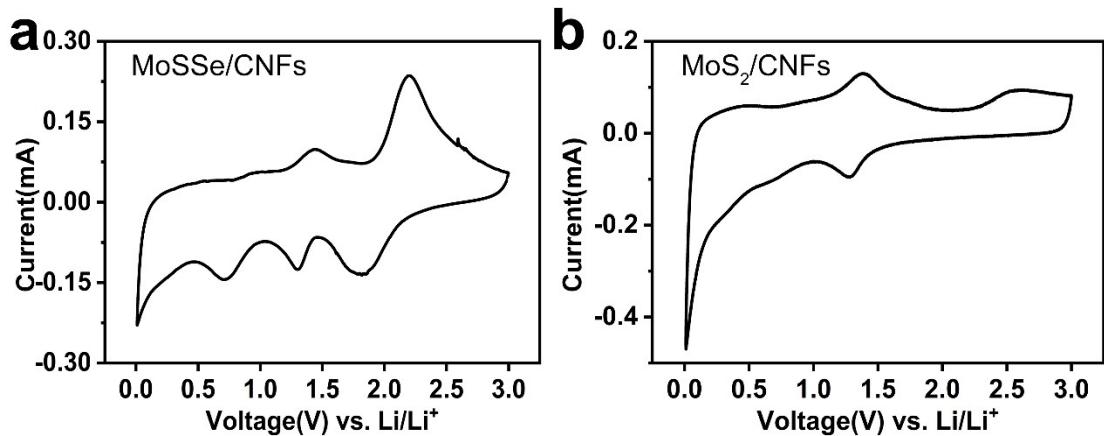
**Figure S6.** N<sub>2</sub> adsorption – desorption isotherm of MoSSe/CNFs,  $\text{MoS}_2/\text{CNFs}$  and  $\text{MoSe}_2/\text{CNFs}$ .



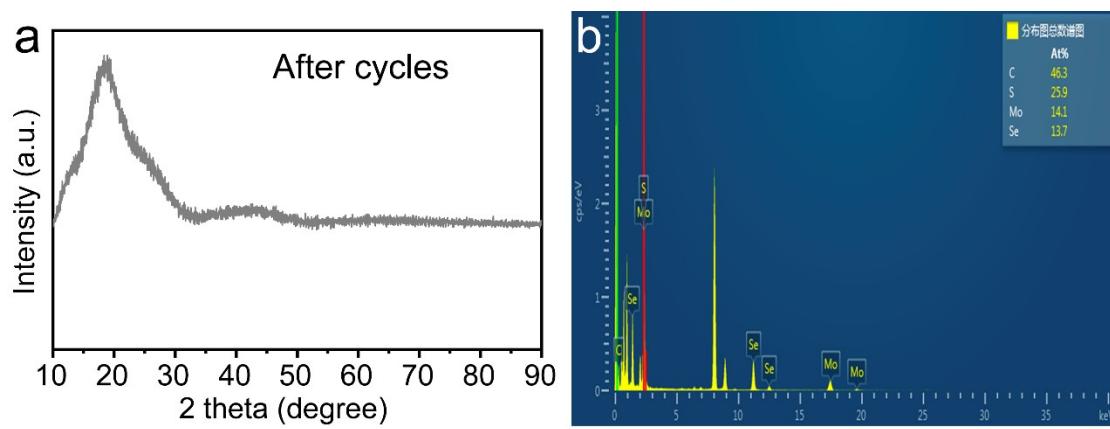
**Figure S8.** a) CV curves at  $0.1 \text{ mV s}^{-1}$  the second cycle of MoSSe/CNFs, MoS<sub>2</sub>/CNFs and MoSe<sub>2</sub>/CNFs. b) Comparison graph of peak currents for MoSSe/CNFs, MoS<sub>2</sub>/CNFs and MoSe<sub>2</sub>/CNFs.



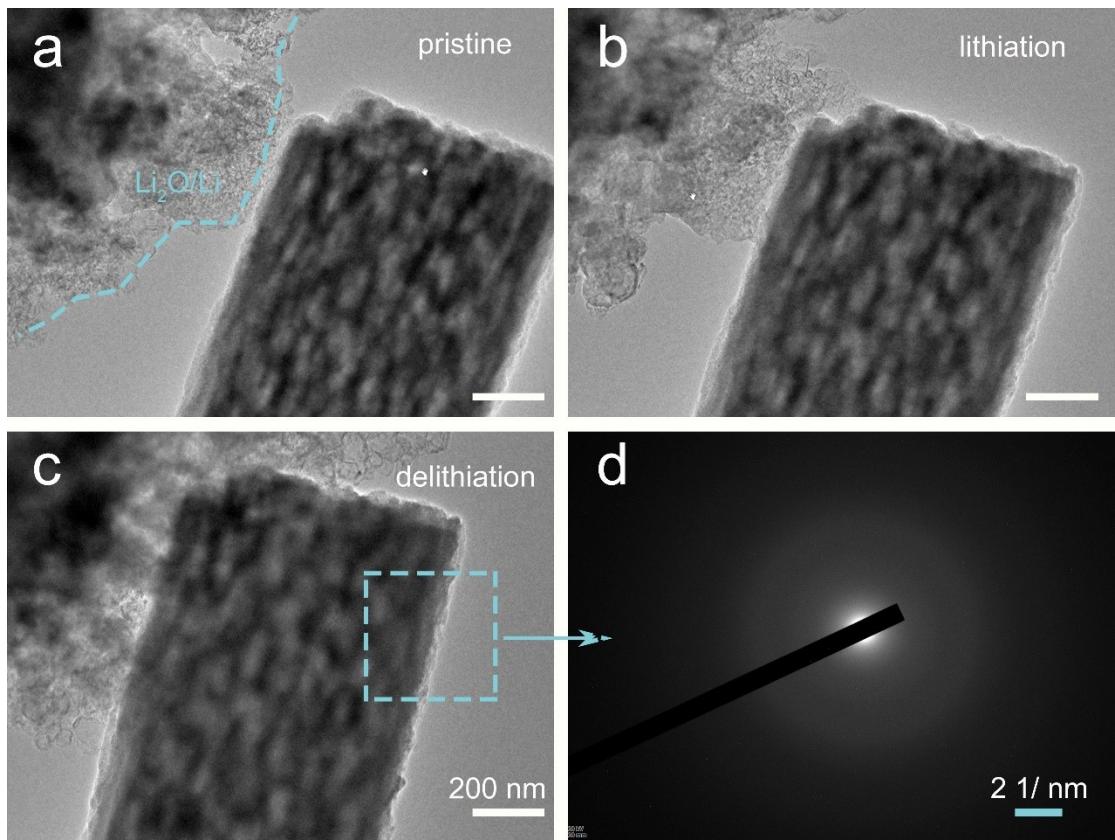
**Figure S9.** a) CV curves of  $\text{MoS}_2/\text{CNFs}$  at  $0.1 \text{ mV s}^{-1}$  scan rate. b) CV curves of  $\text{MoSe}_2/\text{CNFs}$  at  $0.1 \text{ mV s}^{-1}$  scan rate.



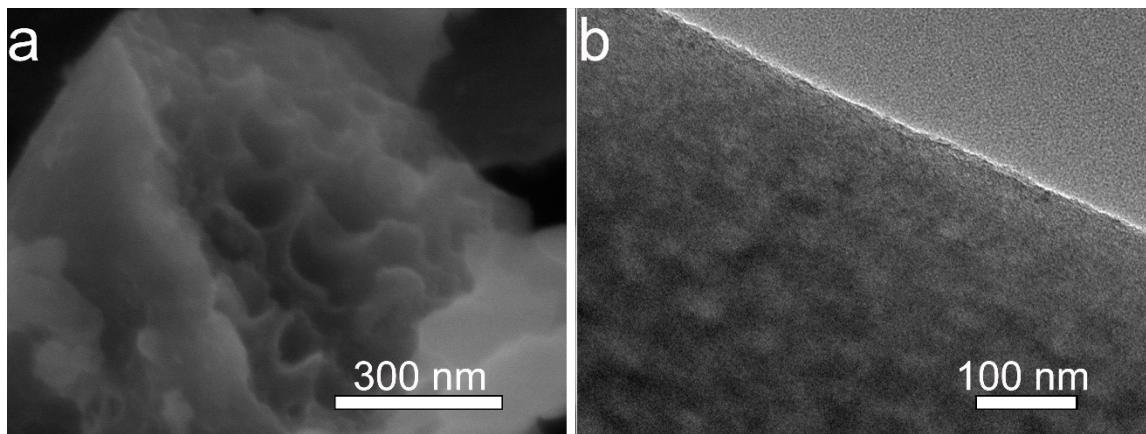
**Figure S10.** a) CV curves of  $\text{MoSSe}/\text{CNFs}$  at  $0.2 \text{ mV s}^{-1}$  scan rate after 200 cycles at  $5 \text{ A g}^{-1}$ . b) CV curves of  $\text{MoS}_2/\text{CNFs}$  at  $0.2 \text{ mV s}^{-1}$  scan rate after 200 cycles at  $5 \text{ A g}^{-1}$ .



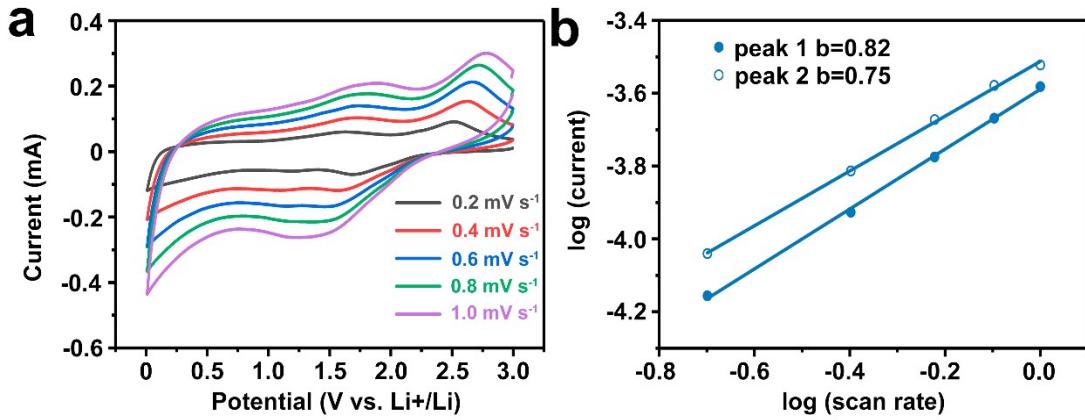
**Figure S11.** a) Elemental compositions of  $\text{MoSSe}/\text{CNFs}$  at fully delithiated to 3 V versus  $\text{Li}^+/\text{Li}$  by EDS analysis. b) XRD patterns of  $\text{MoSSe}/\text{CNFs}$  electrode after cycling.



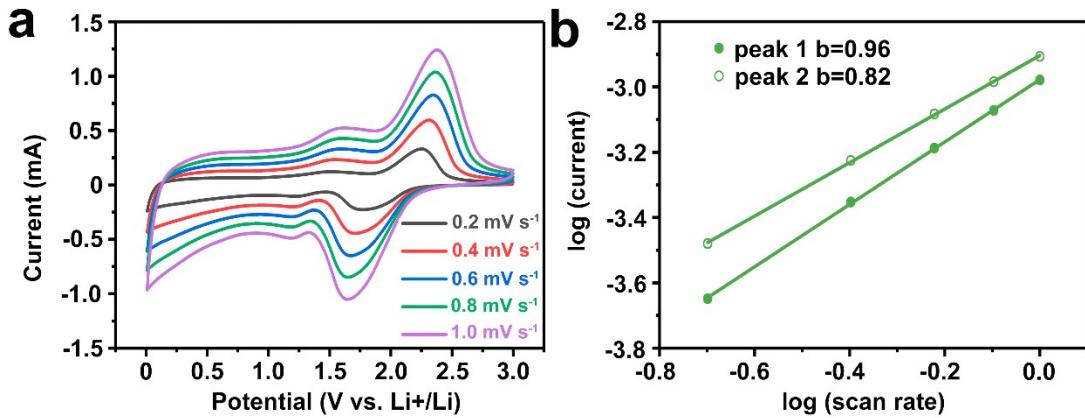
**Figure S12.** a-c) TEM images of MoSSe/CNFs during in situ lithiation/delithiation processes in TEM. d) Selected area electron diffraction (SAED) patterns for after first cycle.



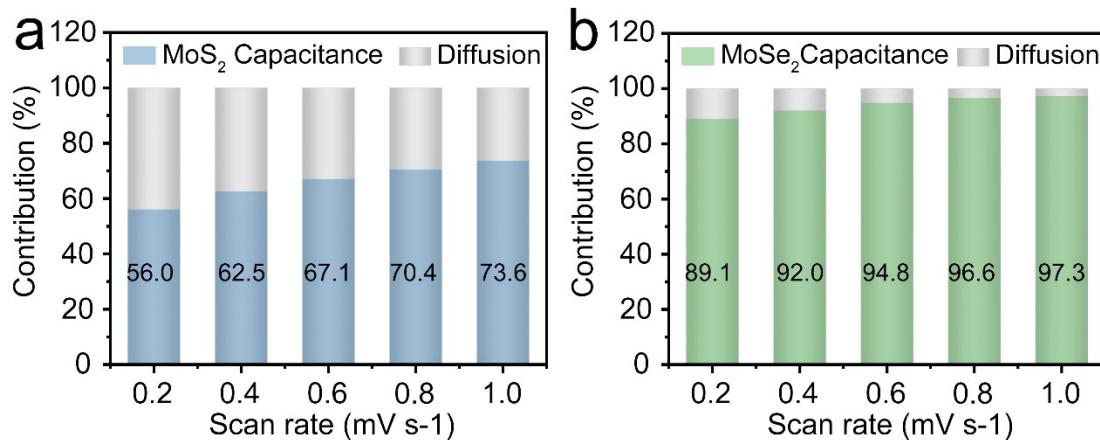
**Figure S13.** a) SEM, b) TEM images of MoSSe/CNFs electrode after cycling.



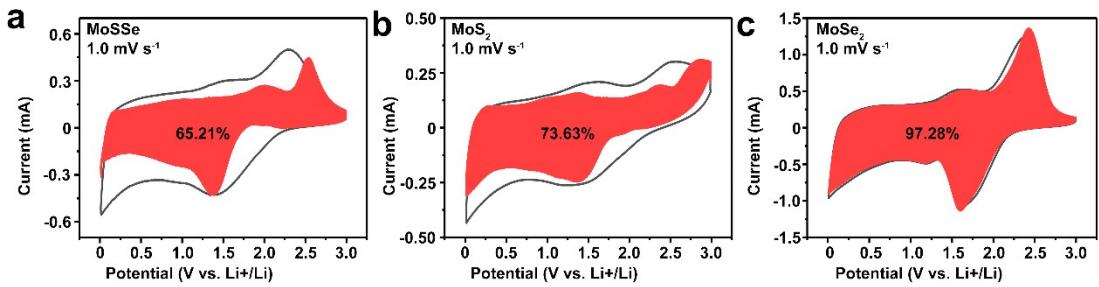
**Figure S14.** a) CV curves of MoS<sub>2</sub>/CNFs at scan rates from 0.2 to 1.0 mV s<sup>-1</sup>. b) Corresponding liner relationship between log ( $i$ ) and log ( $v$ ) of different peaks.



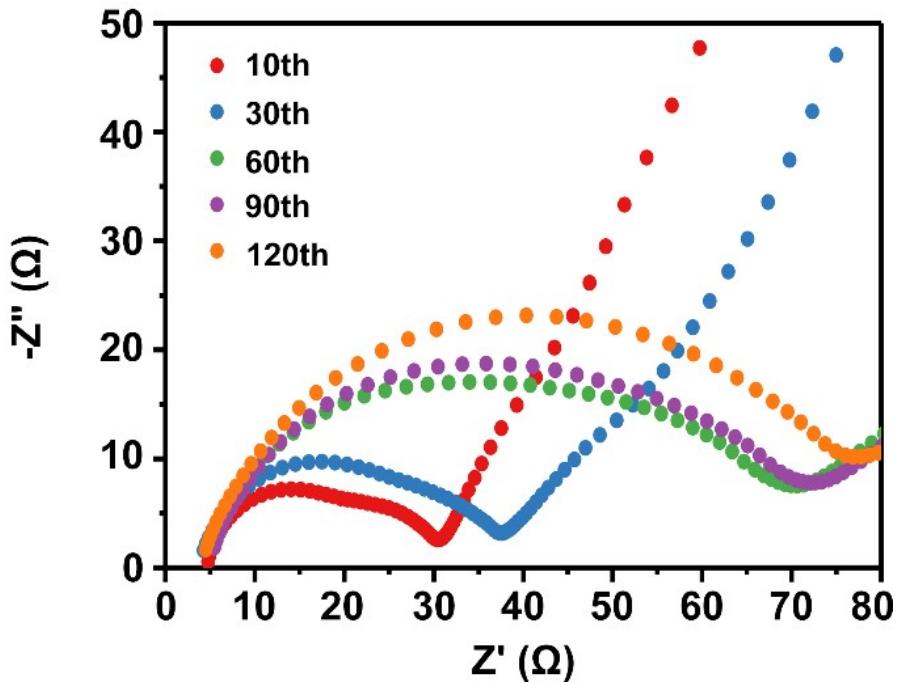
**Figure S15.** a) CV curves of MoSe<sub>2</sub>/CNFs at scan rates from 0.2 to 1.0 mV s<sup>-1</sup>. b) Corresponding liner relationship between log ( $i$ ) and log ( $v$ ) of different peaks.



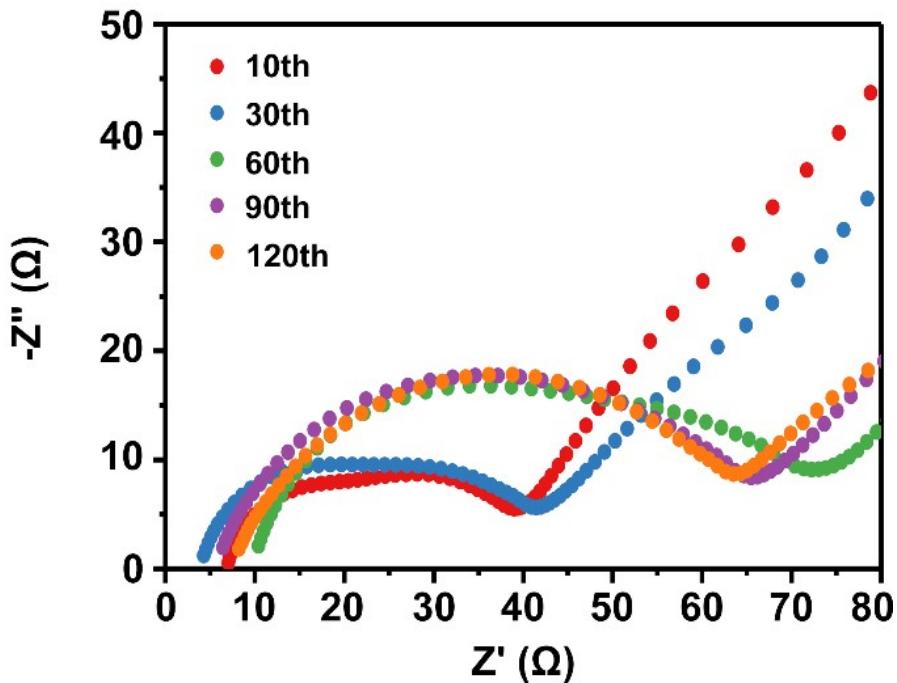
**Figure S16.** Contribution ratio of the capacitive process at different scan rates for a) MoS<sub>2</sub>, and b) MoSe<sub>2</sub>.



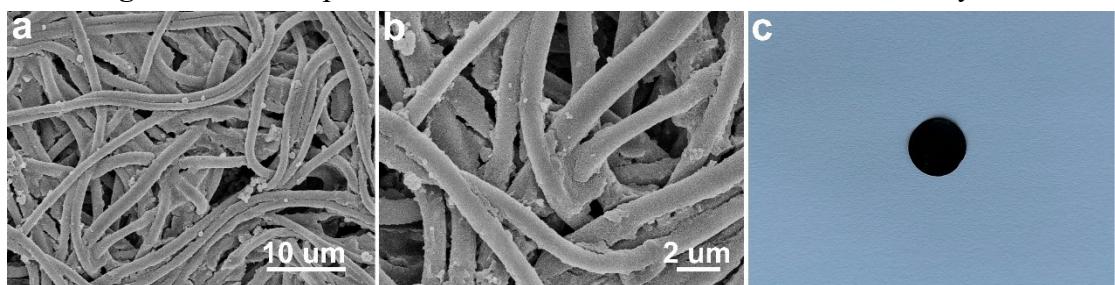
**Figure S17.** CV curves of the capacitive contribution at 1.0 mV s<sup>-1</sup>.



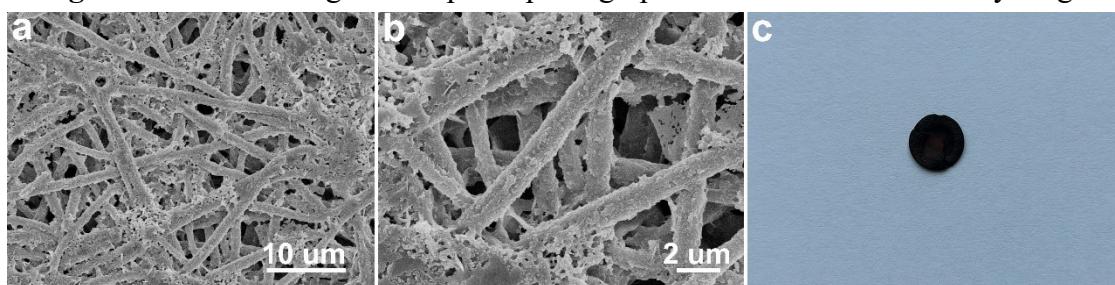
**Figure S18.** EIS spectra of MoS<sub>2</sub>/CNFs electrodes with different cycles.



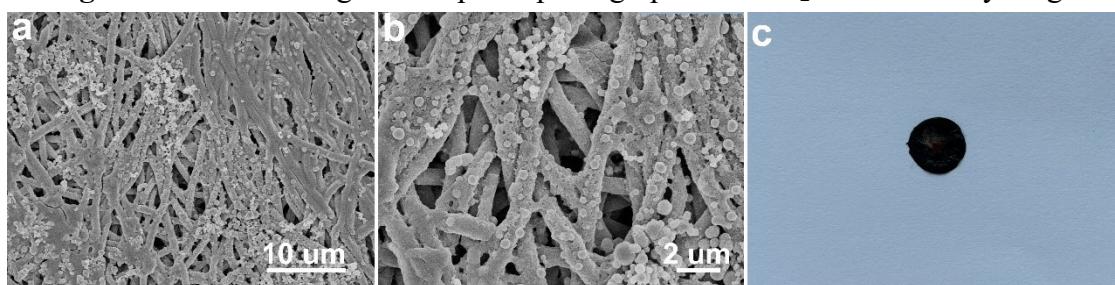
**Figure S19.** EIS spectra of MoSe<sub>2</sub>/CNFs electrodes with different cycles.



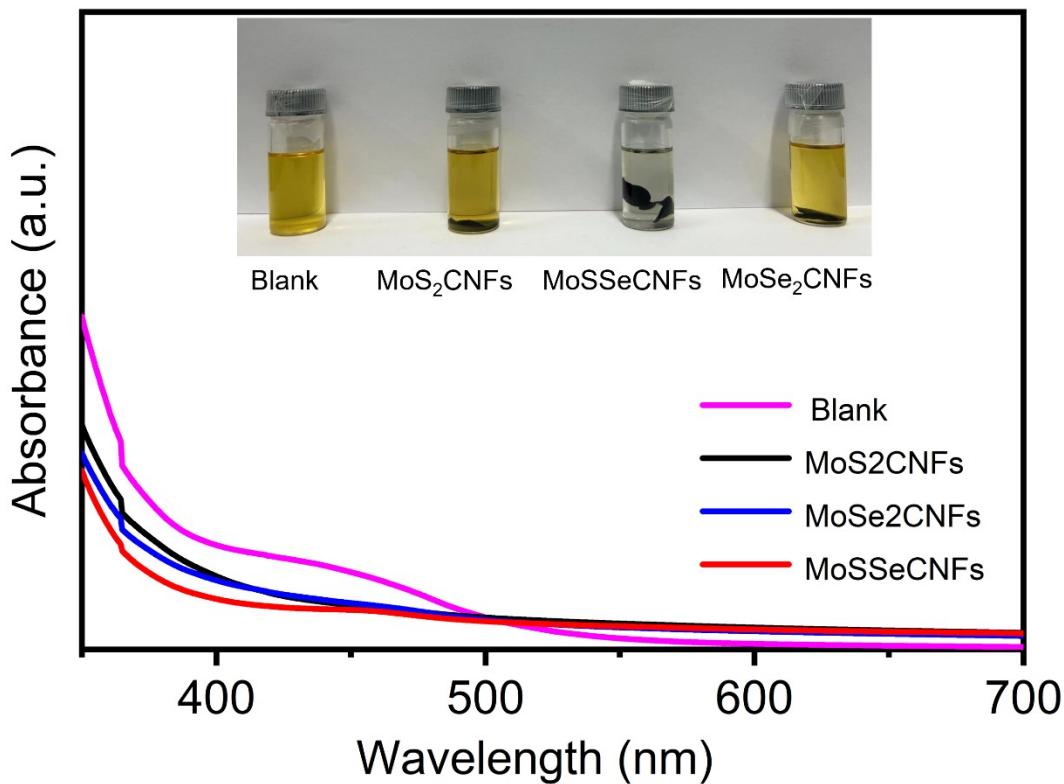
**Figure S20.** SEM images and optical photographs of MoSSe/CNFs after cycling.



**Figure S21.** SEM images and optical photographs of MoS<sub>2</sub>/CNFs after cycling.



**Figure S22.** SEM images and optical photographs of MoSe<sub>2</sub>/CNFs after cycling.



**Figure S23.** UV-Vis spectra of polysulfide solution upon adsorption by different sorbents.

Table S1. Raman spectra parameters of as-prepare products.

Products	D1 band	D3 band	D4 band	G band	I <sub>D1</sub> /I <sub>G</sub>
MoSSe/CNFs	1356	1532	1201	1601	1.42
MoSe <sub>2</sub> /CNFs	1321	1435		1593	1.25
MoS <sub>2</sub> /CNFs	1359	1515		1599	1.31

Table S2. The comparison of molybdenum- or selenide-based or sulfide-based anode materials recently.

Materials	Rate performance	Cyclic performance	Reference
CoP-C@MoS <sub>2</sub> /C	945.5 mAh g <sup>-1</sup> at 0.1 A g <sup>-1</sup> 484.9 mAh g <sup>-1</sup> at 0.1 A g <sup>-1</sup>	460 at 5 A g <sup>-1</sup> for 2000 cycles	[1]
CoS <sub>2</sub> @NC-400	1024.6 mAh g <sup>-1</sup> at 0.2 A g <sup>-1</sup> 463.3 mAh g <sup>-1</sup> at 2 A g <sup>-1</sup>	767.6 at 0.5 A g <sup>-1</sup> for 500 cycles	[2]
NiS/SnO <sub>2</sub> /MOF	932 mAh g <sup>-1</sup> at 0.05 A g <sup>-1</sup> 400 mAh g <sup>-1</sup> at 2 A g <sup>-1</sup>	430 at 2 A g <sup>-1</sup> for 1000 cycles	[3]
MXene@MoS <sub>2</sub>	817 mAh g <sup>-1</sup> at 0.2 A g <sup>-1</sup> 717 mAh g <sup>-1</sup> at 10 A g <sup>-1</sup>	877 at 1 A g <sup>-1</sup> for 70 cycles	[4]
MoS <sub>2</sub> /Fe <sub>2</sub> O <sub>3</sub> @CNF-3	1060 mAh g <sup>-1</sup> at 0.05 A g <sup>-1</sup> 443 mAh g <sup>-1</sup> at 5 A g <sup>-1</sup>	559.74 at 1 A g <sup>-1</sup> for 500 cycles	[5]
Cu <sub>2</sub> S@NSC	610.4 mAh g <sup>-1</sup> at 0.1 A g <sup>-1</sup> 387.6 mAh g <sup>-1</sup> at 5 A g <sup>-1</sup>	512.7 at 1 A g <sup>-1</sup> for 1000 cycles	[6]

NbSe <sub>2</sub> @PPy-2	819 mAh g <sup>-1</sup> at 0.1 A g <sup>-1</sup> 361 mAh g <sup>-1</sup> at 4 A g <sup>-1</sup>	670 at 0.5 A g <sup>-1</sup> for 210 cycles	[7]
MoO <sub>2</sub> /Cu <sub>2-x</sub> Se@C	667.5 mAh g <sup>-1</sup> at 0.1 A g <sup>-1</sup> 285.2 mAh g <sup>-1</sup> at 5 A g <sup>-1</sup>	480.9 at 2 A g <sup>-1</sup> for 500 cycles	[8]
MoSe <sub>2</sub> /rGO	770 mAh g <sup>-1</sup> at 0.1 A g <sup>-1</sup> 560 mAh g <sup>-1</sup> at 2 A g <sup>-1</sup>	732.9 at 1 A g <sup>-1</sup> for 300 cycles	[9]
MoO <sub>2</sub> /N-MCNTs	833.4 mAh g <sup>-1</sup> at 0.5 A g <sup>-1</sup> 523.7 mAh g <sup>-1</sup> at 3 A g <sup>-1</sup>	507.8 at 1 A g <sup>-1</sup> for 500 cycles	[10]
MoSSe/CNFs	996.9 mAh g <sup>-1</sup> at 0.2 A g <sup>-1</sup> 616.8 mAh g <sup>-1</sup> at 10 A g <sup>-1</sup>	750 at 5 A g <sup>-1</sup> for 950 cycles	This work

Table S3. Values of R<sub>s</sub>, R<sub>f</sub> and R<sub>ct</sub> obtained from the fitting date.

Electrodes	R <sub>s</sub> (Ω)	R <sub>f</sub> (Ω)	R <sub>ct</sub> (Ω)
MoSSe/CNFs	4.546	36.24	102.4
MoSe <sub>2</sub> /CNFs	2.252	48.64	237.4
MoS <sub>2</sub> /CNFs	10.65	32.08	418.1

### References:

- [1] Y. Xia, T. Yang, Z. Wang, T. Mao, Z. Hong, J. Han, D.L. Peng, G. Yue, Van der Waals forces between S and P ions at the CoP-C@MoS<sub>2</sub>/C heterointerface with enhanced lithium/sodium storage, *Adv. Funct. Mater.* 33 (2023) 2302830. <https://doi.org/10.1002/adfm.202302830>.
- [2] J. Xu, P. Ye, Y. Cheng, L. Ji, Y. Wei, Y. Chen, Meta-organic framework-based CoS<sub>2</sub> nitroge-doped carbon for high-performance lithium storage, *Energy Technol-Ger* 11 (2023) 2201452. <https://doi.org/10.1002/ente.202201452>.
- [3] N. Zhang, Q. Meng, H. Wu, X. Hu, M. Zhang, A. Zhou, Y. Li, Y. Huang, L. Li, F. Wu, R. Chen, Co-MOF as stress-buffered architecture: an engineering for improving the performance of NiS/SnO<sub>2</sub> heterojunction in lithium storage, *Adv. Energy Mater.* (2023). <https://doi.org/10.1002/aenm.202300413>.
- [4] H. Tan, L. Zhang, K. Gao, L. Sun, Y. Zhang, F. Xie, Few-layer MoS<sub>2</sub> nanosheets vertically supported on Ti<sub>3</sub>C<sub>2</sub>-MXene sheets promoting lithium storage performance, *Dalton T.* 52 (2023) 16413-16420. <https://doi.org/10.1039/d3dt01963b>.
- [5] X. Chen, Q. Zhang, H. Wang, L. Wang, H. Wang, Y. Zeng, MoS<sub>2</sub> nanoflowers implanted in nitrogen-doped carbon fibers with Fe<sub>2</sub>O<sub>3</sub> nanoparticles decorated for enhanced lithium storage performance, *J. Alloys Compd.* 963 (2023). <https://doi.org/10.1016/j.jallcom.2023.171195>.
- [6] T. Li, D. Zhao, M. Shi, T. Wang, Q. Yin, Y. Li, J. Qi, F. Wei, Y. Sui, MOF-derived N,S Co-doped carbon matrix-encapsulated Cu<sub>2</sub>S nanoparticles as high-performance lithium-ion battery anodes: a joint theoretical and experimental study, *J. Mater. Chem. A* 11 (2023) 1461-1472. <https://doi.org/10.1039/d2ta08539a>.
- [7] B.-H. Kang, S. Shin, K. Nam, J. Bae, J.-M. Oh, S.-M. Koo, H. Sohn, S.-H. Park, W.H. Shin, Exfoliated NbSe<sub>2</sub> nanosheet@polypyrrole hybrid nanocomposites as a high performance anode of lithium-ion batteries, *J. Mater. Chem. A* 11 (2023) 19083-19090. <https://doi.org/10.1039/d3ta01335a>.
- [8] M. Zhong, X. Guo, L. Li, Y.-W. Li, K. Zhao, H. Peng, X. Zhang, Hetero-phase MoO<sub>2</sub>/Cu<sub>2-x</sub>Se nanocomposites distributed in porous octahedral carbon networks for high-performance lithium

- storage, ACS Appl. Nano Mater. 6 (2023) 20018-20027. <https://doi.org/10.1021/acsanm.3c03824>.
- [9] W. Wang, J.-Y. Chen, J. Ouyang, H. Yin, A.-J. Li, L. Chen, J.-L. Huang, Y.-C. Zhu, G.-Y. Li, Z.-H. Hou, Spray pyrolysis-derived W-doped MoSe<sub>2</sub>/rGO paper-like microspheres: optimization of microstructure and mesostructure for enhanced lithium storage, Rare Met. 43 (2024) 3019-3031. <https://doi.org/10.1007/s12598-024-02662-4>.
- [10] Z. Wang, X. Chen, D. Wu, T. Zhang, G. Zhang, S. Chu, B. Qian, S. Tao, Strong metal oxide-support interaction in MoO<sub>2</sub>/N-doped MCNTs heterostructure for boosting lithium storage performance, J. Colloid Interface Sci. 650 (2023) 247-256. <https://doi.org/10.1016/j.jcis.2023.06.192>.