

## Supplementary Information

### Constructing robust and freestanding MXene/Si@C core-shell nanofibers via coaxing electrospinning for high performance Li-ion batteries

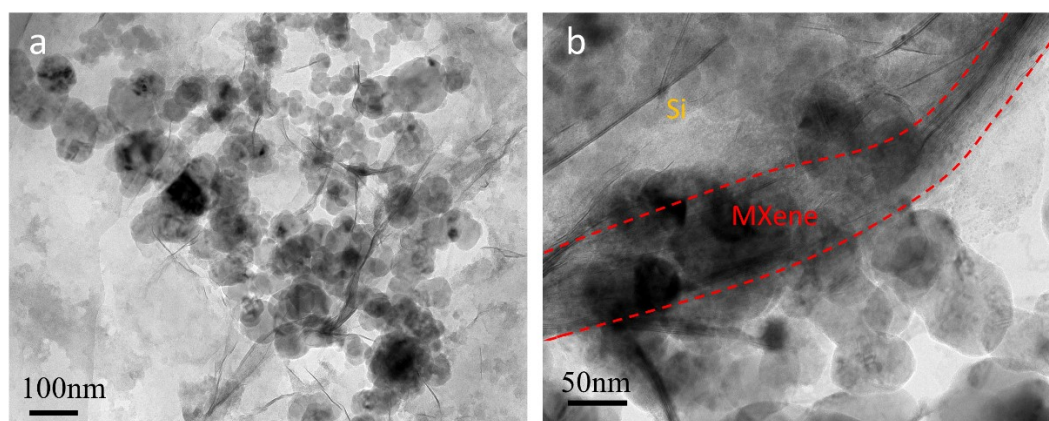
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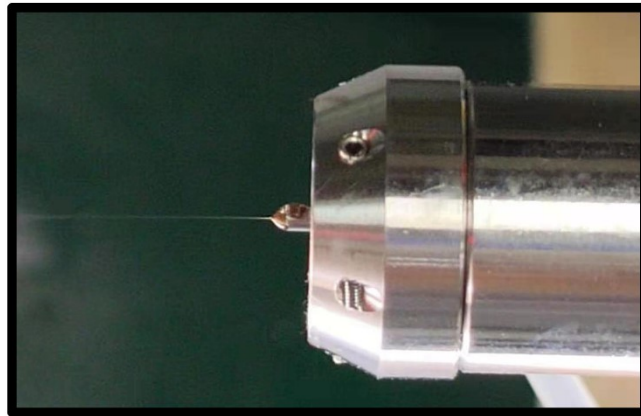
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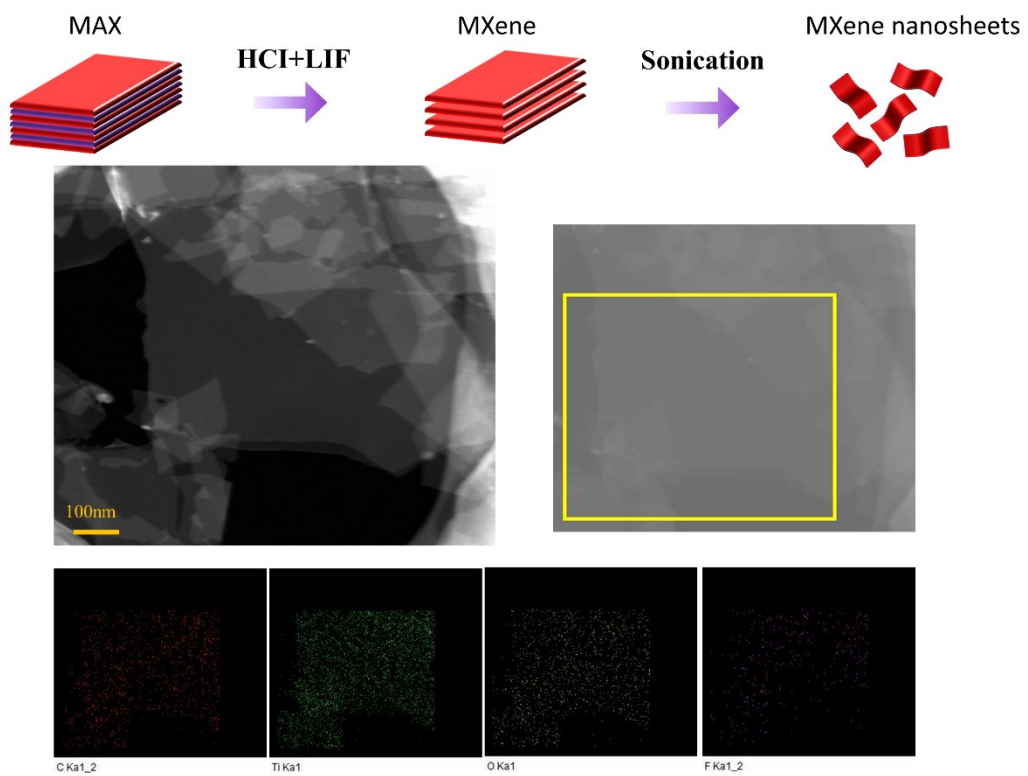
### Supplementary Figures



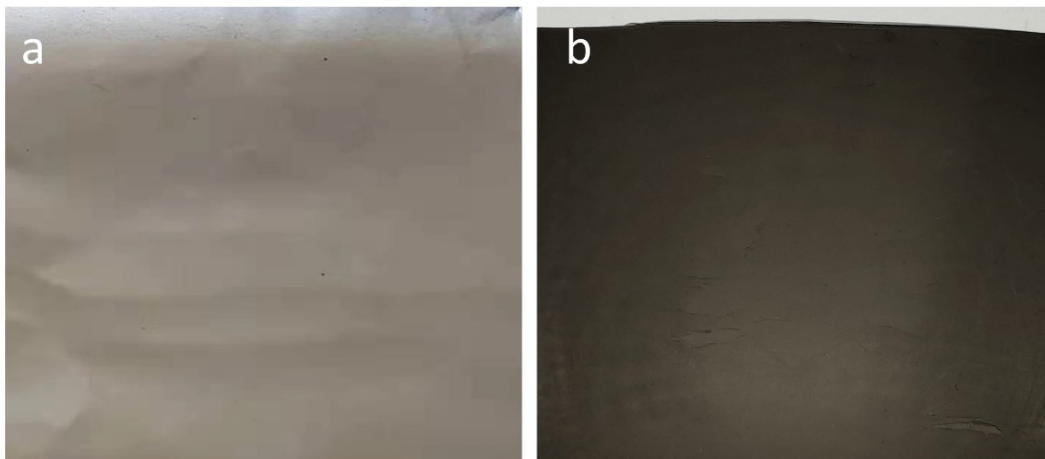
**Figure S1.** a) The SEM of MXene/Si after stirring 1h in DMF/acetone (1:1=w:w). b) Magnified SEM of MXene/Si contact part.



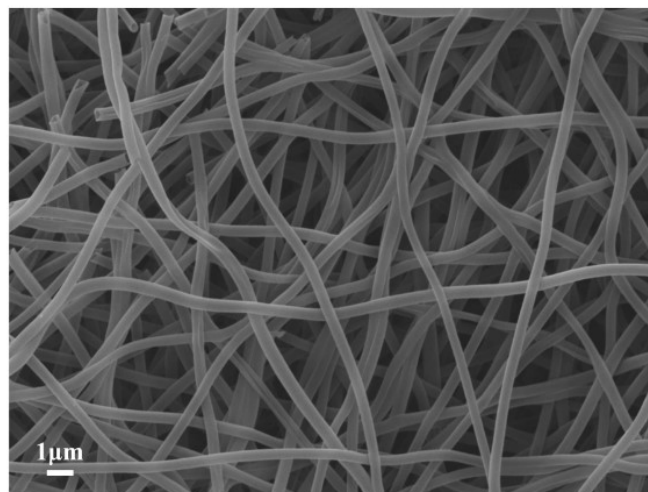
**Figure S2.** The coaxing nozzle and Taylor core during electrospinning.



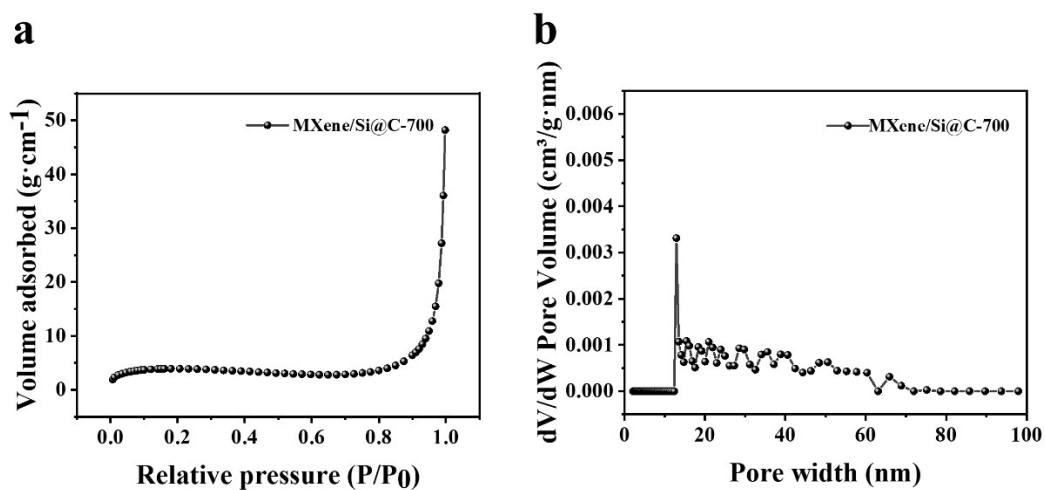
**Figure S3.** Synthesis of MXene and elemental mapping of MXene.



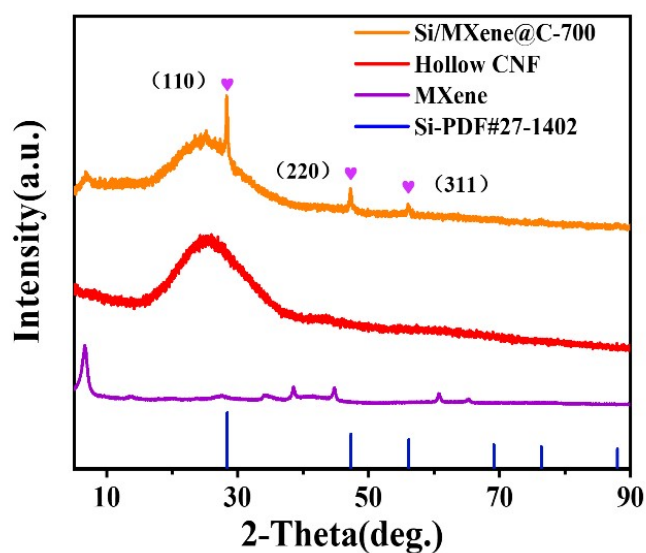
**Figure S4.** a) Electrospun MXene/Si/PMMA@PAN precursor film. b) MXene/Si@C film after carbonization at 700°C.



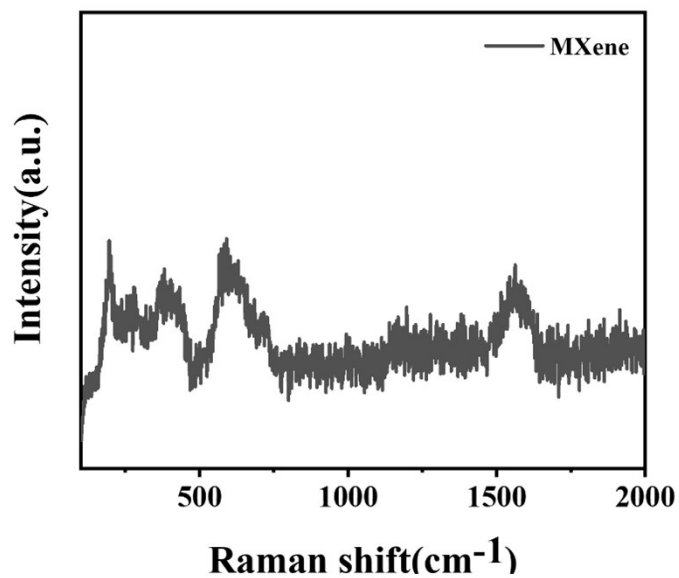
**Figure S5.** SEM of hollow carbon nanofibers carbonized at 700°C.



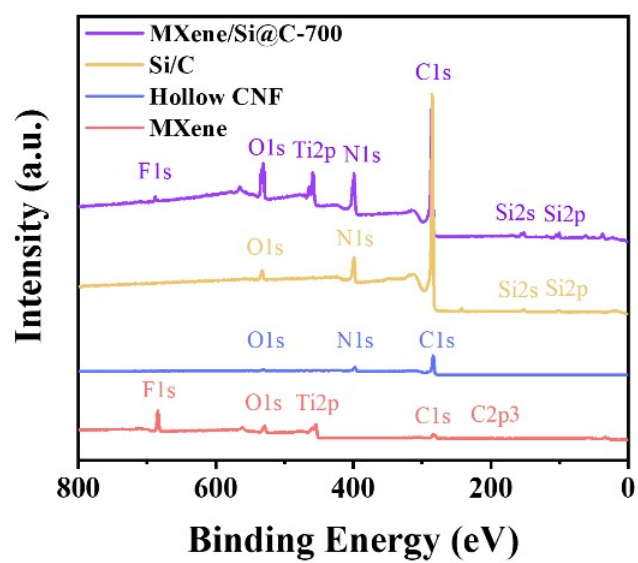
**Figure S6.** (a) Nitrogen adsorption–desorption isotherms of MXene/Si@C-700 (b) Corresponding pore diameter distributions.



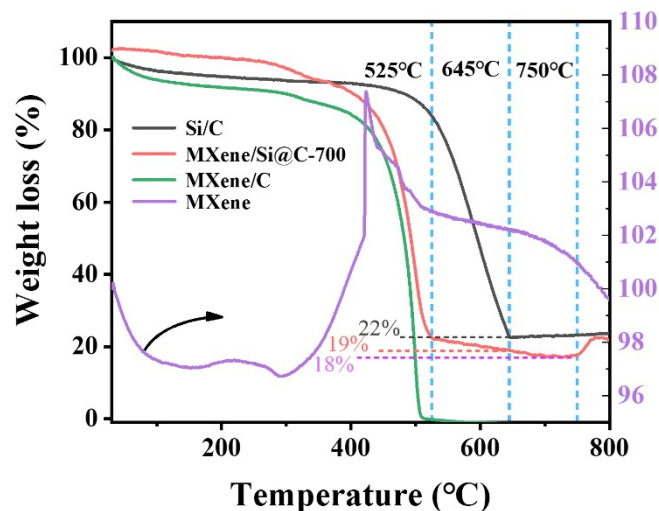
**Figure S7.** XRD pattern of MXene/Si@C-700, Hollow CNF and MXene.



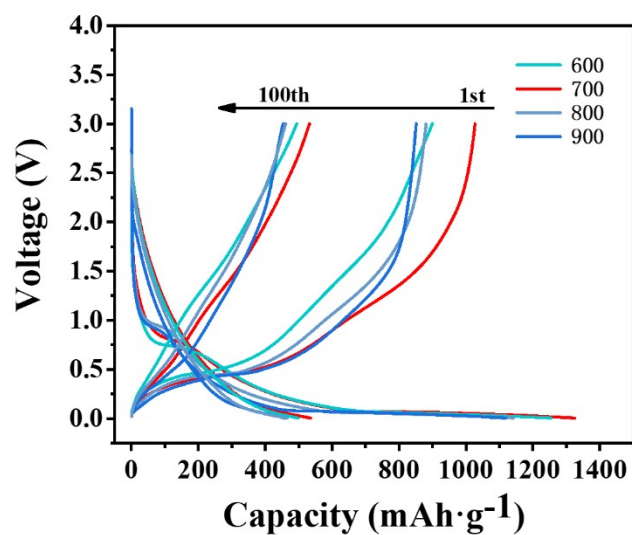
**Figure S8.** Raman spectrum of MXene.



**Figure S9.** a) Typical XPS profile of the MXene/Si@C-700, Si/C, hollow CNF and MXene.

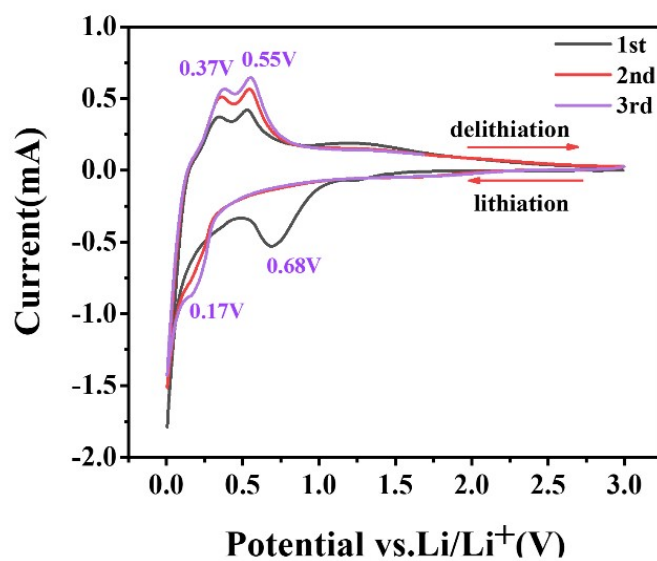


**Figure S10.** TGA curves of MXene/Si@C-700, Si/C nanofiber, MXene/C nanofiber and MXene.

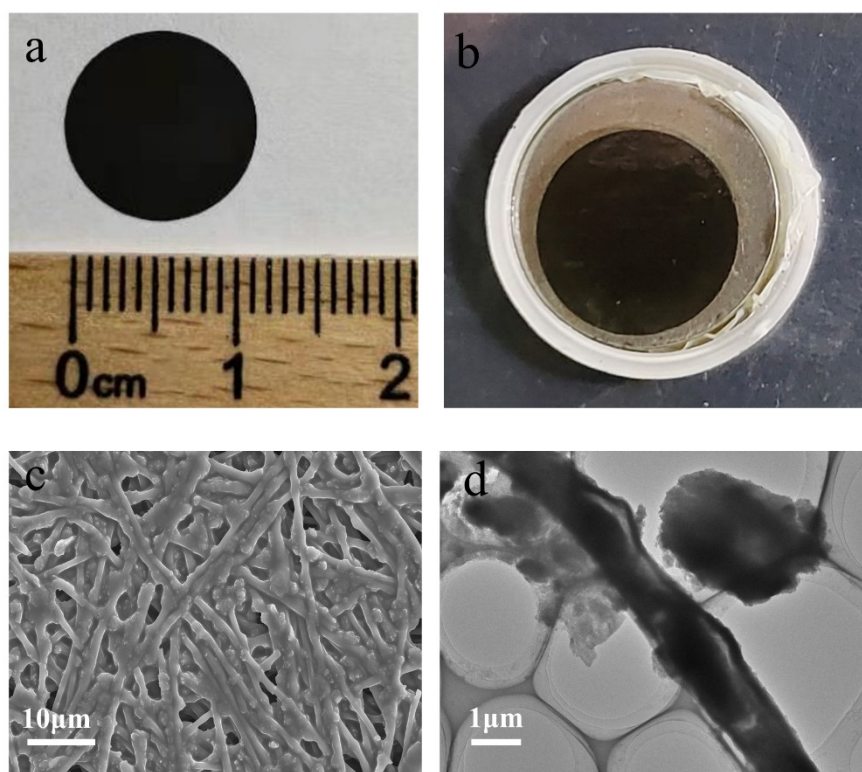


**Figure S11.** The initial and 100th galvanostatic charge/discharge profiles of MXene/Si@C carbonized at different temperatures (600, 700, 800, 900°C).

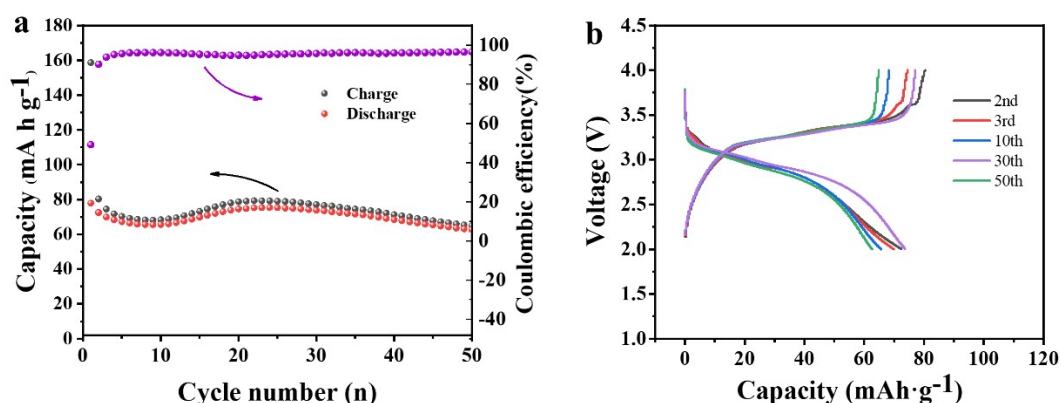




**Figure S12.** Initial three CV curves of Si/C electrode.



**Figure S13.** a) MXene/Si@C-700 electrode. b) MXene/Si@C-700 electrode after 1000 cycles at  $1 \text{ A g}^{-1}$  c) SEM of MXene/Si@C-700 nanofibers after 1000 cycles at  $1 \text{ A g}^{-1}$  d) TEM of MXene/Si@C-700 nanofibers after 1000 cycles at  $1 \text{ A g}^{-1}$



**Figure S14.** a) Cycling performance of LFP||MXene/Si@C-700 full cell at 0.1A g<sup>-1</sup>. b) Corresponding galvanostatic charge/discharge profiles

In order to demonstrate the potential in practical application, full cells were constructed with MXene/Si@C-700 as anode and LiFePO<sub>4</sub> as cathode. As show in Figure S14 a,b, the full cell shows a voltage platform of about 3.2V with an initial reversible capacity of 80mAh g<sup>-1</sup> and 67 mAh g<sup>-1</sup> after 50 cycles. The gravimetric energy densities of the full cell based on the LFP||MXene/Si@C-700 is calculated to be 180Wh kg<sup>-1</sup> in the initial cycle and 150Wh kg<sup>-1</sup> in the 50th cycle.<sup>1</sup>

The relative low energy densities is due to low ICE in the full cell, and it can be improved by prelithiation<sup>2</sup> or selecting proper electrolyte additives<sup>3</sup>. The coulombic efficiency keeps stable from the second cycle, which is ascribed to the stable core-shell structure and integrated conductive network.

## Supplementary Table

**Table S1. Lithium storage performance comparison between this work and previously reported Si-based and MXene-based anode materials.**

Si content (%)	Current density (A g <sup>-1</sup> )	Capacity (mAh g <sup>-1</sup> )	ICE (%)	Utilization efficiency (%)	Ref.
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<b>Si core/C shell</b>	50	0.137	1305	87.5	55	4
<b>Si/CNF@Graphene</b>	29	0.1	1313	79.4	59	5
<b>AG@Si@C</b>	6.4	0.1	448	81.0	37	6
<b>Si p-NS@TNSs</b>	85.6	0.1	1498	80.2	41	1
<b>Si core/C shell</b>	9.9	0.05	596	61.6	67	7
<b>Si@MXene</b>	70	0.2	1797	74.7	58	8
<b>Si/MXene</b>	38.3	0.1	1316	61.1	70	9
<b>MXene/Si@SiOx@C</b>	72.8	0.84	1674	81.3	48	10
<b>This Work</b>	18	0.1	1083	78.4	86	

## Supporting References

1. M. Xia, B. Chen, F. Gu, L. Zu, M. Xu, Y. Feng, Z. Wang, H. Zhang, C. Zhang and J. Yang, Ti<sub>3</sub>C<sub>2</sub>T<sub>x</sub> MXene Nanosheets as a Robust and Conductive Tight on Si Anodes Significantly Enhance Electrochemical Lithium Storage Performance, *ACS Nano*, 2020, 14, 5111-5120.
2. L. Guo, C. Xin, J. Gao, J. Zhu, Y. Hu, Y. Zhang, J. Li, X. Fan, Y. Li, H. Li, J. Qiu and W. Zhou, The Electrolysis of Anti-Perovskite Li<sub>2</sub> OHCl for Prelithiation of High-Energy-Density Batteries, *Angew Chem Int Ed Engl*, 2021, 60, 13013-13020.
3. M. Ge, C. Cao, G. M. Biesold, C. D. Sewell, S. M. Hao, J. Huang, W. Zhang, Y. Lai and Z. Lin, Recent Advances in Silicon-Based Electrodes: From Fundamental Research toward Practical Applications, *Adv Mater*, 2021, 33, 2004577.
4. T. H. Hwang, Y. M. Lee, B.-S. Kong, J.-S. Seo and J. W. Choi, Electrospun Core-Shell Fibers for Robust Silicon Nanoparticle-Based Lithium Ion Battery Anodes, *Nano Letters*, 2012, 12, 802-807.
5. M.-S. Wang, W.-L. Song and L.-Z. Fan, Three-Dimensional Interconnected Network of Graphene-Wrapped Silicon/Carbon Nanofiber Hybrids for Binder-Free Anodes in Lithium-Ion Batteries, *ChemElectroChem*, 2015, 2, 1699-1706.
6. H. Chen, Z. Wang, X. Hou, L. Fu, S. Wang, X. Hu, H. Qin, Y. Wu, Q. Ru, X. Liu and S. Hu, Mass-producible method for preparation of a carbon-coated graphite@plasma nano-silicon@carbon composite with enhanced performance as lithium ion battery anode, *Electrochimica Acta*, 2017, 249, 113-121.
7. B.-S. Lee, S.-B. Son, K.-M. Park, J.-H. Seo, S.-H. Lee, I.-S. Choi, K.-H. Oh and W.-R. Yu, Fabrication of Si core/C shell nanofibers and their electrochemical performances as a lithium-ion battery anode, *Journal of Power Sources*, 2012, 206, 267-273.
8. Y. Yan, X. Zhao, H. Dou, J. Wei, Z. Sun, Y. S. He, Q. Dong, H. Xu and X. Yang, MXene Frameworks Promote the Growth and Stability of LiF-Rich Solid-Electrolyte Interphases on Silicon Nanoparticle Bundles, *ACS Appl Mater Interfaces*, 2020, 12, 18541-18550.
9. X. Hui, R. Zhao, P. Zhang, C. Li, C. Wang and L. Yin, Low-Temperature Reduction Strategy Synthesized Si/Ti<sub>3</sub>C<sub>2</sub> MXene Composite Anodes for High-Performance Li-Ion Batteries, *Adv. Energy Mater.*, 2019, 9, 1901065.
10. Y. Zhang, Z. Mu, J. Lai, Y. Chao, Y. Yang, P. Zhou, Y. Li, W. Yang, Z. Xia and S. Guo, MXene/Si@SiO<sub>x</sub>@C Layer-by-Layer Superstructure with Autoadjustable Function for Superior Stable Lithium Storage, *ACS Nano*, 2019, 13, 2167-2175.