Arginine modification of hybrid cobalt/nitrogen Ti$_3$C$_2$T$_x$ MXene and its application as a sulfur host for lithium-sulfur batteries

Miao Zhang[1], Kaiyu Zhang[1], Wei Wei[1], Hongxin Yuan[2], Jingjing Chang[1], Yue Hao[1]

[1]Academy of Advanced Interdisciplinary Research, Xidian University, Xi'an 710071, Shaanxi, China.
[2]School of Materials Science and Engineering, Nanyang Technological University, Singapore 639798, Singapore.

Correspondence to: Prof. Jingjing Chang, Academy of Advanced Interdisciplinary Research, Xidian University, 266 Xinglong Section of Xifeng Road, Xi'an 710126, Shaanxi, China. E-mail: jjingchang@xidian.edu.cn; Dr. Miao Zhang, Academy of Advanced Interdisciplinary Research, Xidian University, 266 Xinglong Section of Xifeng Road, Xi'an 710126, Shaanxi, China. E-mail: miaozhang@xidian.edu.cn
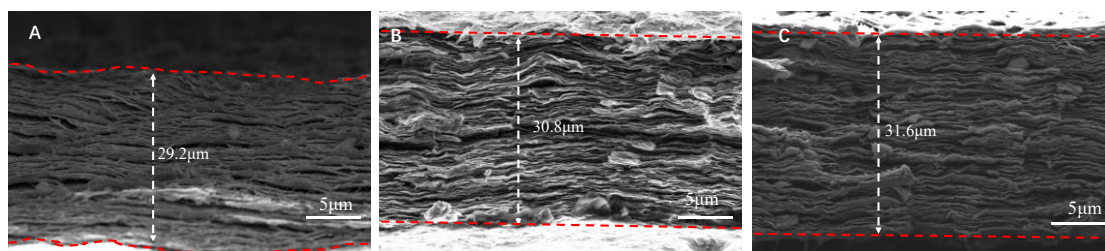
Figure S1 Cross sectional SEM images of Co-N@Ti$_3$C$_2$T$_{X-Ser}$, Co-N@Ti$_3$C$_2$T$_{X-Lys}$ and Co-N@Ti$_3$C$_2$T$_{X-Arg}$.
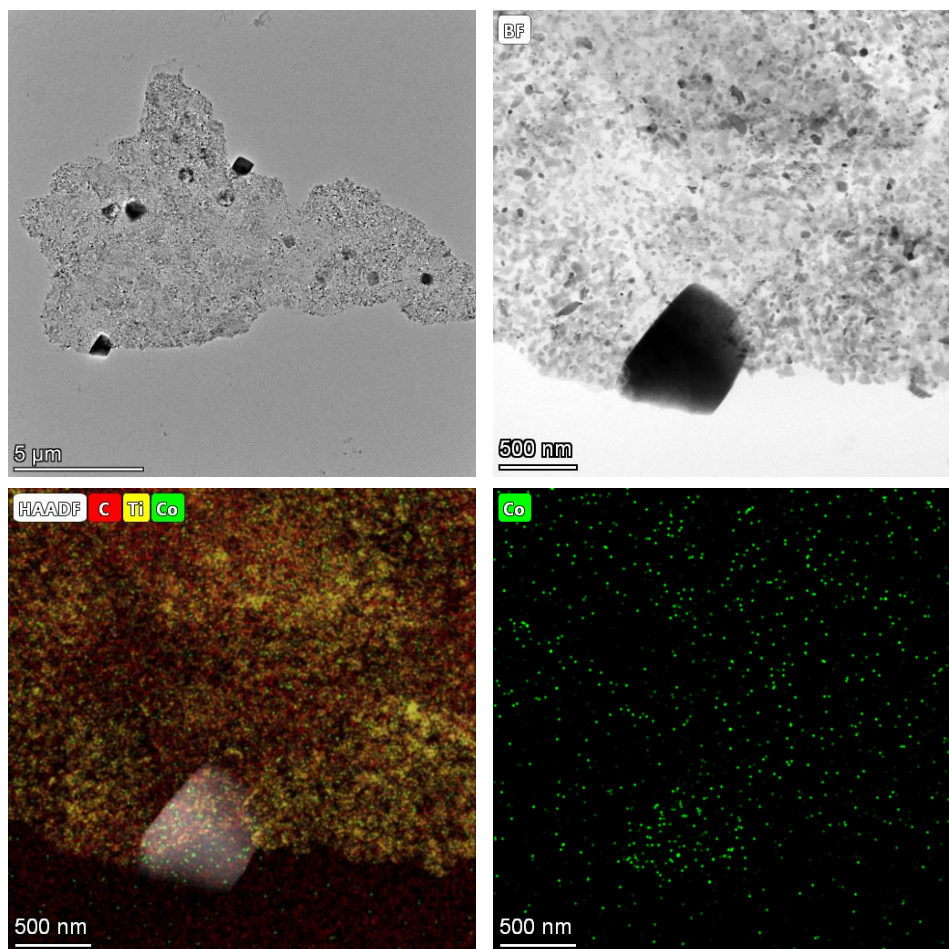

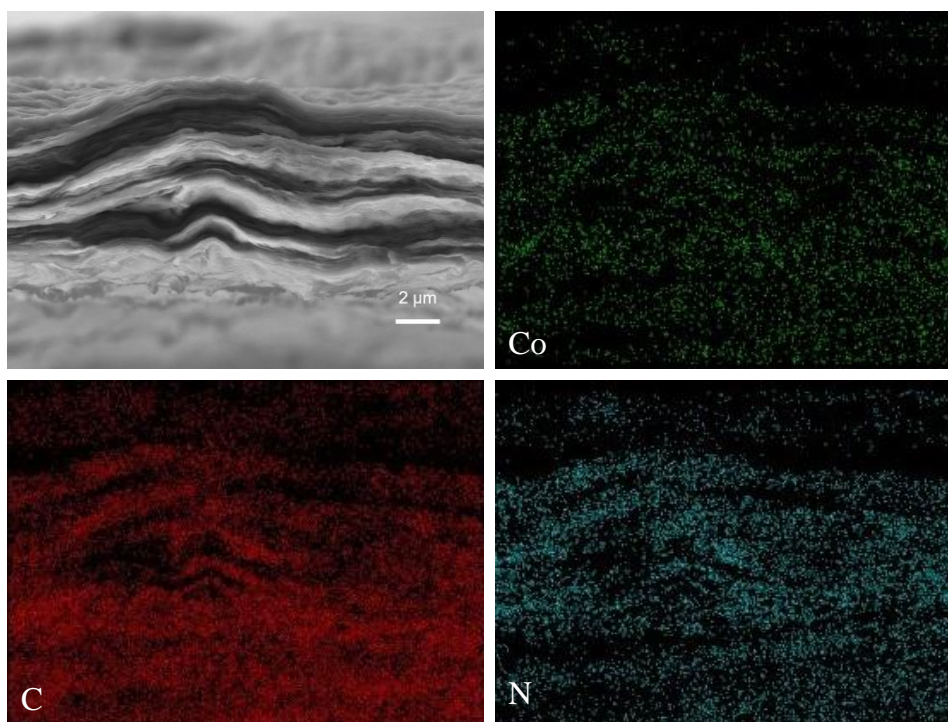Figure S2 The TEM images and elemental mappings of the Co-N@Ti$_3$C$_2$T$_{x-Arg}$

Figure S3 SEM image and EDS spectrum mapping: C, Co and N elemental distribution of Co-N@Ti$_3$C$_2$T$_{X-Ser}$ composite.
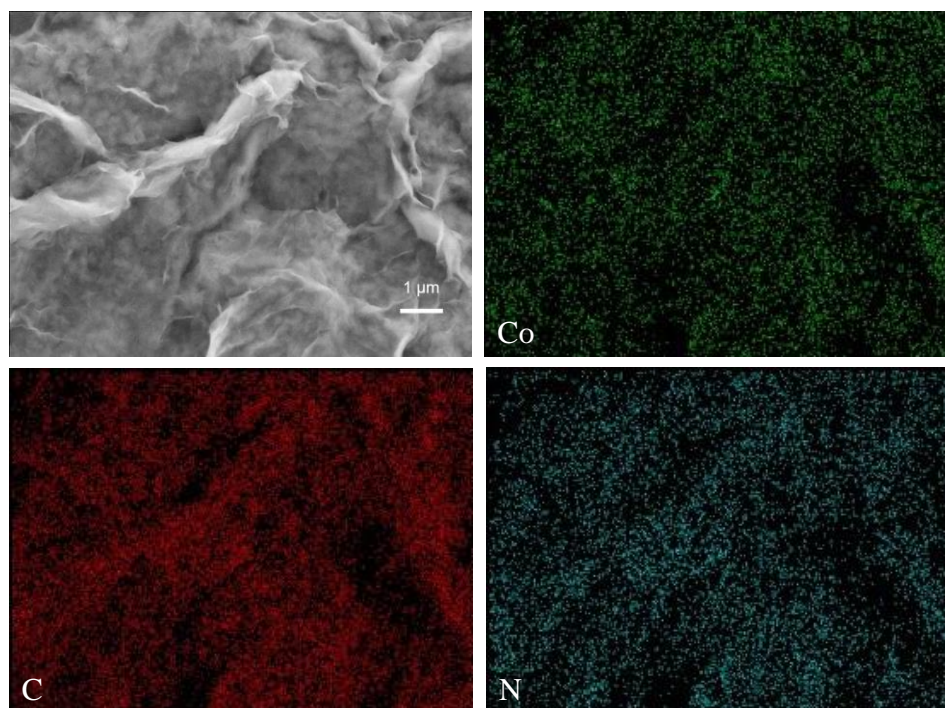

Figure S4 SEM image and EDS spectrum mapping: C, Co and N elemental distribution of Co-N@Ti$_3$C$_2$T$_{X-Lysr}$ composite.
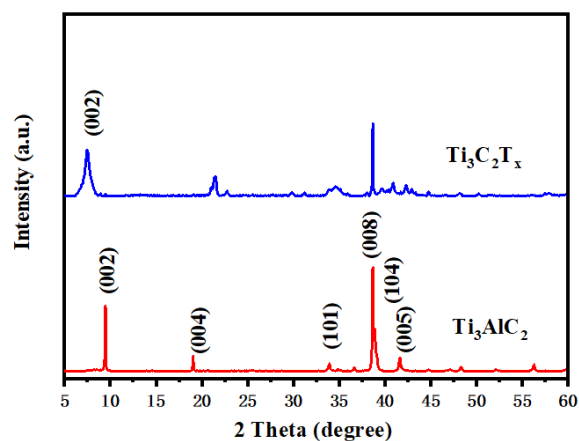
Figure S5 XRD pattern of $Ti_3Al_2T_x$ and $Ti_3C_2T_x$.
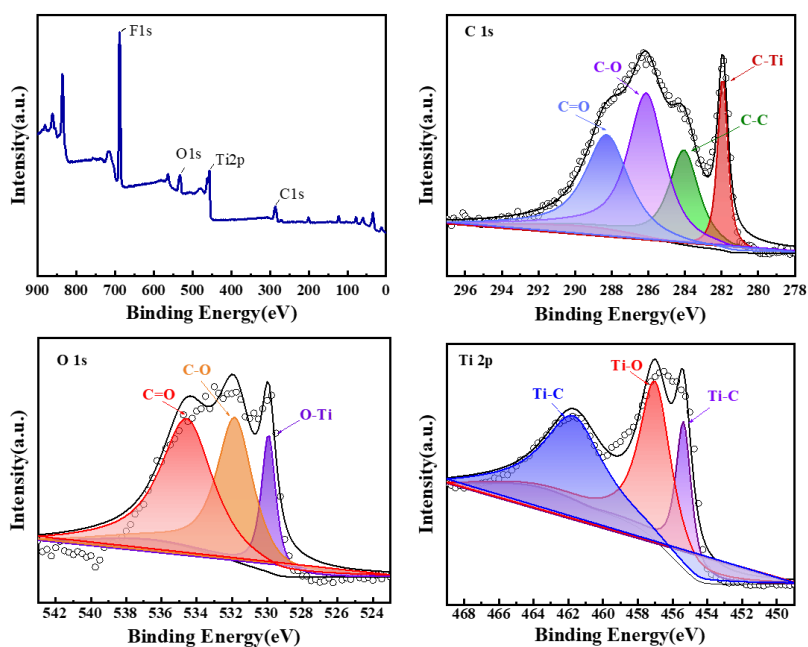
Figure S6 a) XPS study for $Ti_3C_2T_x$ composites of the total scale. b) C 1s XPS spectrum of $Ti_3C_2T_x$. c) O 1s spectrum of $Ti_3C_2T_x$. d)Ti 2p spectrum of $Ti_3C_2T_x$.
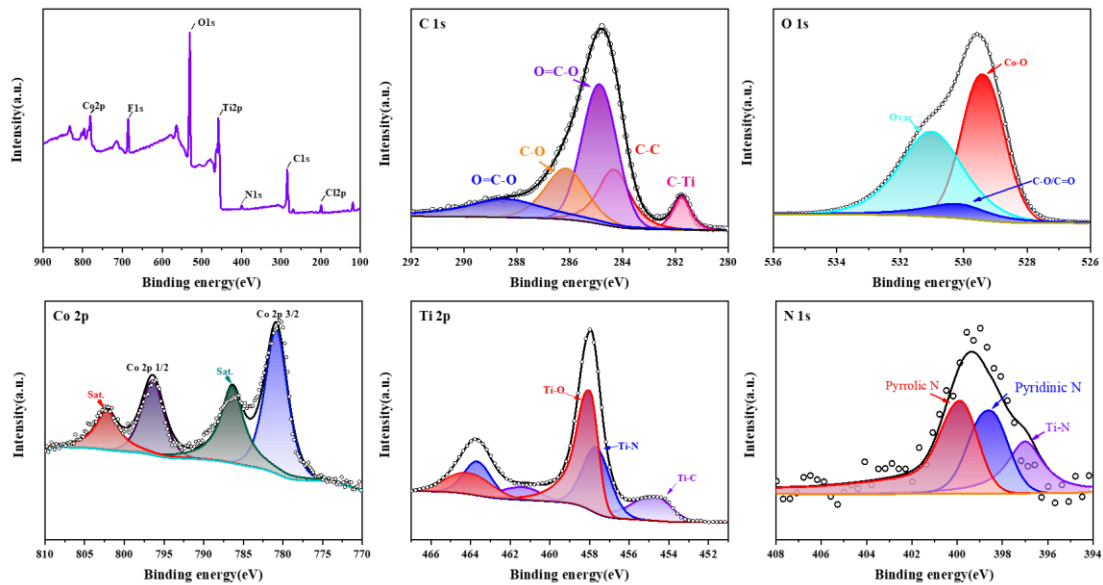
Figure S7 a) XPS study for Co-N@Ti$_3$C$_2$T$_{x-Ser}$ composites of the total scale. b) C 1s XPS spectrum of Co-N@Ti$_3$C$_2$T$_{x-Ser}$ composites. c) O 1s spectrum of Co-N@Ti$_3$C$_2$T$_{x-Ser}$ composites. d) Co 2p spectrum of Co-N@Ti$_3$C$_2$T$_{x-Ser}$ composites. e) Ti 2p spectrum of Co-N@Ti$_3$C$_2$T$_{x-Ser}$ composites. h) N 1s spectrum of Co-N@Ti$_3$C$_2$T$_{x-Ser}$ composites.
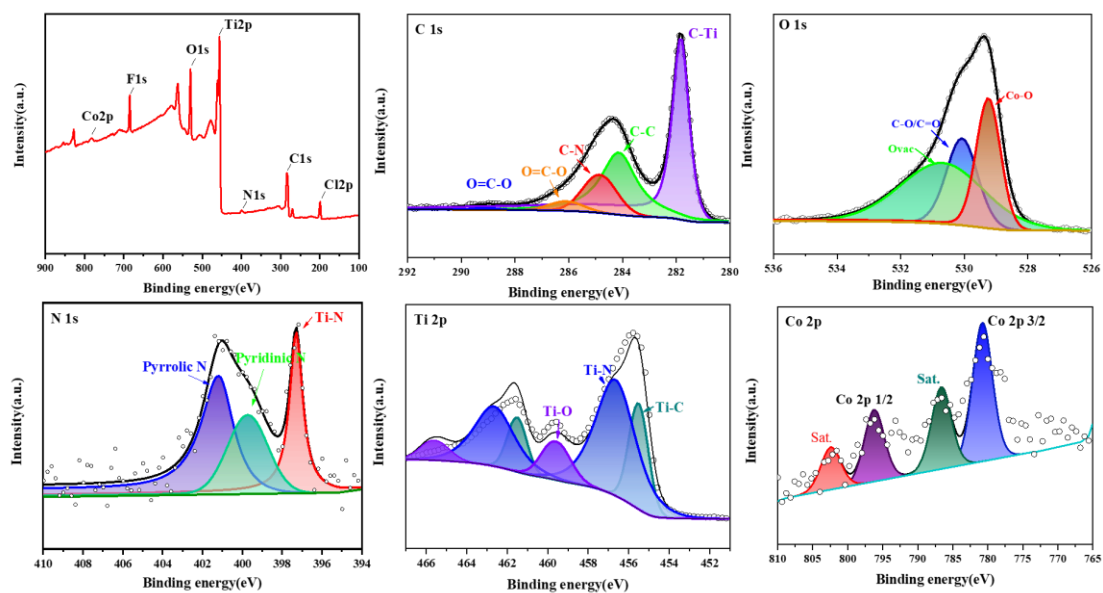
Figure S8 a) XPS study for Co-N@Ti$_3$C$_2$T$_{x-Lys}$ composites of the total scale. b) C 1s XPS spectrum of Co-N@Ti$_3$C$_2$T$_{x-Lys}$ composites. c) O 1s spectrum of Co-N@Ti$_3$C$_2$T$_{x-Lys}$ composites. d) Co 2p spectrum of Co-N@Ti$_3$C$_2$T$_{x-Lys}$ composites. e) Ti 2p spectrum of Co-N@Ti$_3$C$_2$T$_{x-Lys}$ composites. h) N 1s spectrum of Co-N@Ti$_3$C$_2$T$_{x-Lys}$ composites.
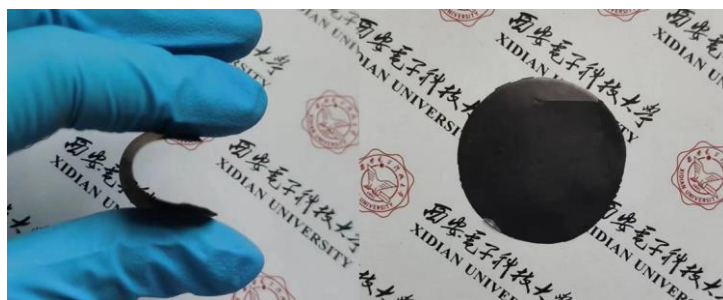
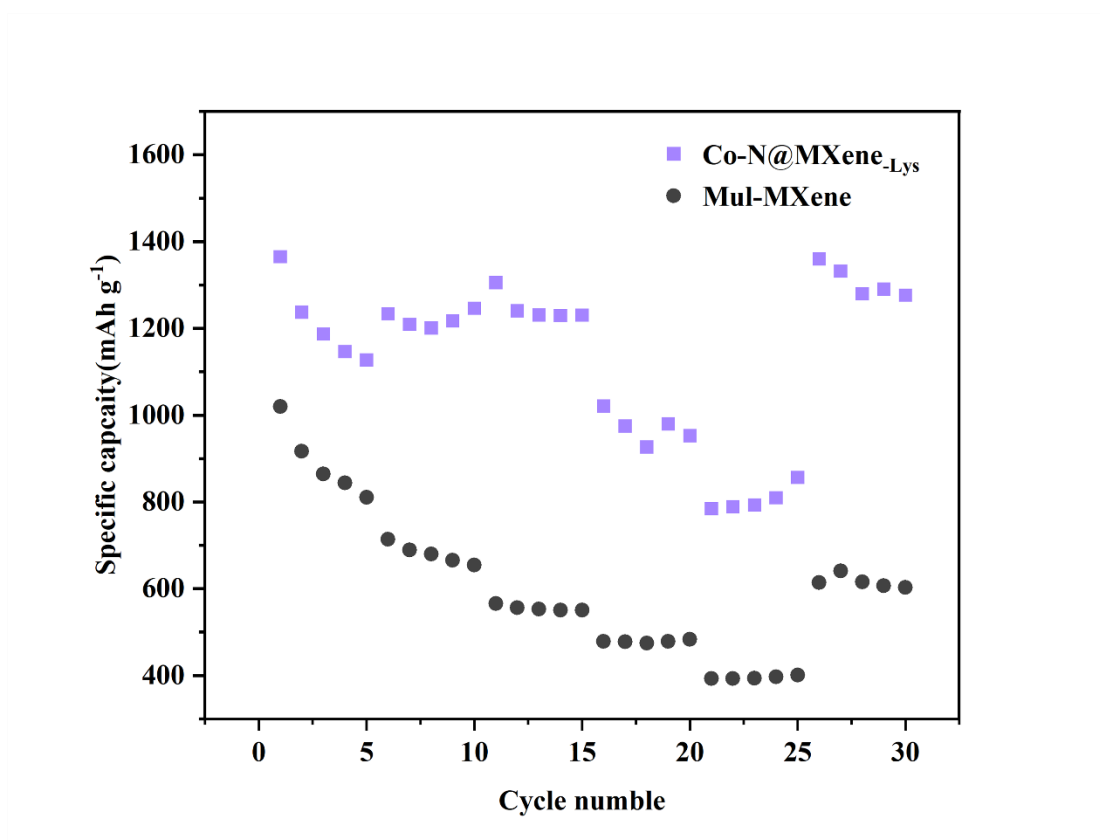Figure S9 the flexible Co-N@Ti$_3$C$_2$T$_{x-Lys}$ film.

Figure S10 The rate capability of Mul-MXene and Co-N@Ti$_3$C$_2$T$_{x-Arg}$ composite
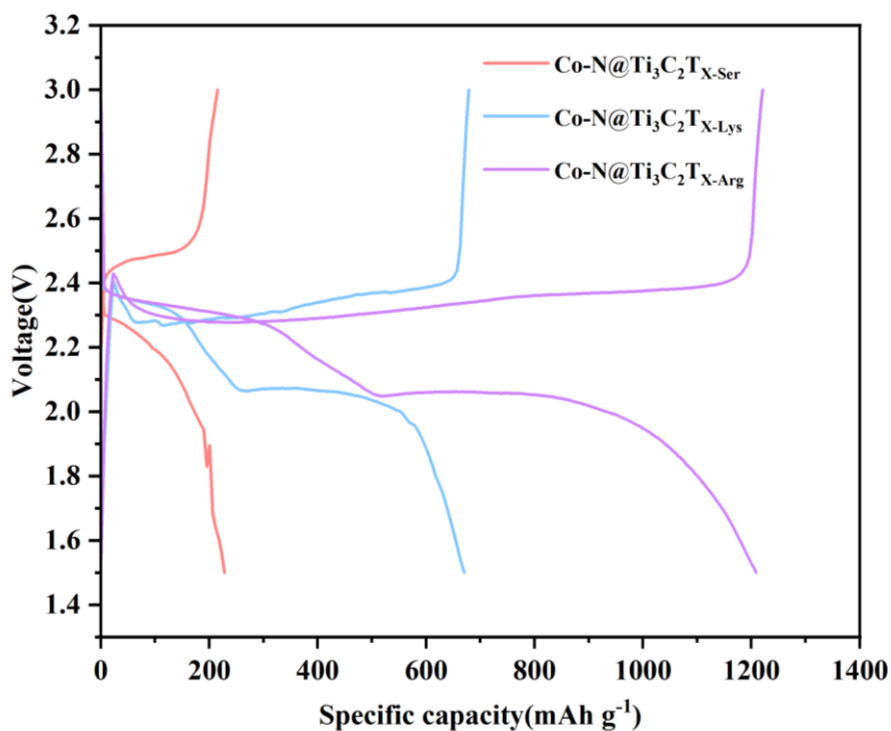
cathode at 0.1, 0.2, 0.5, 1, 2 C.

Figure S11. Discharge–charge curves of the Co-N@$Ti_3C_2T_{X-Ser}$/S, Co-N@$Ti_3C_2T_{X-Lys}$/S, and Co-N@$Ti_3C_2T_{X-Arg}$/S composite electrodes at 0.2 C.
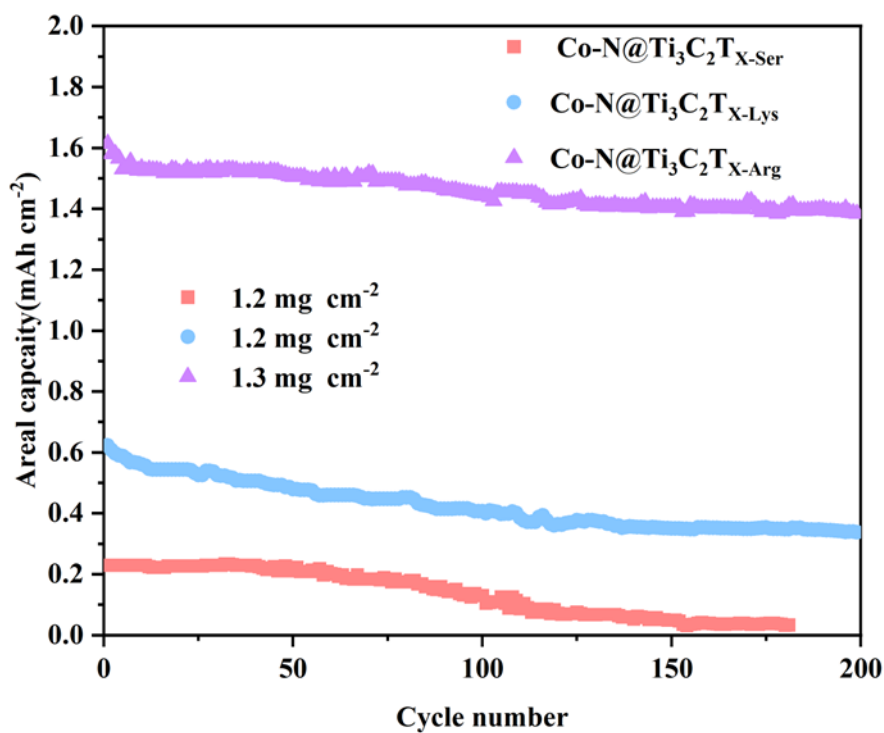

Figure S12 Comparison of areal capacity of Co-N@$Ti_3C_2T_{x-Ser}$/S, Co-N@$Ti_3C_2T_{x-}$

$_{Lys}$/S, and Co-N@Ti$_3$C$_2$T$_{x-Arg}$/S electrode at 0.2 C.

Table S1 Performances and strategies of representative MXene-based Li-S batteries.

Materials	Current density	Initial capacity (mAh g^{-1})	Cycle life/rate capacity	Capacity retention ratio (%)	Ref
TiO$_2$/Ti$_2$C	0.2 C	879.2	rate capacity	/	[1]
Ti$_n$O$_{2n-1}$/MXene	0.2 C	1227	100	81.5	[2]
TiS$_2$/TiO$_2$@MXene	0.2 C	1232	100	86.7	[3]
N-Ti$_3$C$_2$T$_x$	0.2 C	1144	200	83.0%	[4]
TiN@MXene	0.2 C	1185	250	84.1	[5]
Co-N@Ti$_3$C$_2$T$_{X-Arg}$	0.2 C	1314.3	200	83.4	This work

References

[1] Du C, Wu J, Yang P, et al. Embedding S@TiO$_2$ Nanospheres into MXene Layers as High Rate Cyclability Cathodes for Lithium-Sulfur Batteries, Electrochim Acta, 2019, 295: 1067-1074. DOI: 10.1016/j.electacta.2018.11.143.

[2] Xia J, Gao R, Yang Y, et al. Ti$_{(n)}$O$_{(2n-1)}$/MXene Hierarchical Bifunctional Catalyst Anchored on Graphene Aerogel toward Flexible and High-Energy Li-S Batteries, ACS Nano, 2022, 16: 19133-19144. DOI 10.1021/acsnano.2c08246.

[3] Nguyen V P, Park J S, Shim H C, et al. Accelerated Sulfur Evolution Reactions by TiS$_2$/TiO$_2$@MXene Host for High-Volumetric-Energy-Density Lithium-Sulfur Batteries, Adv Funct Mater, 2023, 33: 202303503. DOI 10.1002/adfm.202303503.

[4] Bao W, Liu L, Wang C, et al. Facile Synthesis of Crumpled Nitrogen-Doped MXene Nanosheets as a New Sulfur Host for Lithium-Sulfur Batteries, Adv Energy Mater, 2018, 8: 201702485. DOI 10.1002/aenm.201702485.

[5] Zhang M, Lu Y, Yue Z, et al. Design and Synthesis of Novel Pomegranate-like TiN@MXene Microspheres as Efficient Sulfur Hosts for Advanced Lithium Sulfur Batteries, RSC Adv, 2023, 13: 9322-9332. DOI 10.1039/d3ra00095h.