Supporting Information

Sustainable synthesis of metal compound/carbon composites via coordination chemistry for high-performance lithium-ion batteries

Weicai Zhang^{a,b†}, Xiaomin Lin^{a†}, Yawei Fang^a, Chaowei Yang^a, Mingtao Zheng^{a,c} and Yeru Liang^{a,c}*

^aKey Laboratory for Biobased Materials and Energy of Ministry of Education,

College of Materials and Energy, South China Agricultural University, Guangzhou

510642, P. R. China

^bSongshan Lake Materials Laboratory (SLAB), Dongguan 523808, P. R. China

^cMaoming Branch, Guangdong Laboratory of Lingnan Modern Agriculture, Maoming [†]Equal contribution

*Corresponding author: E-mail: liangyr@scau.edu.cn



Fig. S1 N 1s spectra of CTS, CTS-S and CTS-P.



Fig. S2 XPS spectra of CTS-Ni, CTS-P-Ni and CTS-S-Ni.



Fig. S3 Concentration of Ni in CTS-Ni, CTS-S-Ni and CTS-P-Ni.



Fig. S4 HRTEM image of Ni_3S_2/C .



Fig. S5 SEM images and EDS images of NiFe₂O₄/C, CoNiO₂/C and CoFe₂O₄/C.



Fig. S6 Schematic illustration of lithium storage mechanism in Ni₃S₂/C anode.



Fig. S7 Cycling performances of Ni_3S_2/C and C anodes at the current density of 1.0 A

g⁻¹.



Fig. S8 SEM images of Ni_3S_2/C anode before and after cycling.



Fig. S9 CV curves of $Ni_{12}P_5/C$ anodes at 0.2 mV s⁻¹.



Fig. S10 Rate performance of $Ni_{12}P_5/C$ anode.



Fig. S11 Cycling performance of ZnS/C anode at the current density of 0.05 A g^{-1} .



Fig. S12 Cycling performance of NiFe₂O₄/C anode at the current density of 0.10 A

 g^{-1} .

Anodes	Current density (A g ⁻¹)	Cycle number	Discharge capacity (mAh g ⁻¹)	Ref.
NiS–GNS	0.1	60	887	[1]
NiS@OLC	0.1	100	546	[2]
C⊃NiS-L	60	100	300	[3]
NiS/N-rGO	0.5	100	467	[4]
CSF-NiS/C	0.1	100	411.6	[5]
NiS/G	50	400	481	[6]
NiS _x /rGO-500	0.1	60	1026.0	[7]
NiS@SiO ₂ /graphene	0.1	100	750	[8]
HBC-NiS/C	0.2	100	652	[9]
NiS@NSC	0.1	200	715.9	[10]
Ni ₃ S ₂ /C	0.05	250	1434	This work

Table S1. Comparisons of the cycling performance of Ni_xS_y -based anodes for LIBs.

Anodes	Rate capability/mAh g ⁻¹ (Numbers in parentheses denote current density in mA g ⁻¹)	Ref.
NiS@SiO ₂ /graphene	680 (20), 640 (30), 610 (50), 570 (80), 540 (1200), 500 (1600)	[8]
GeS2@NiS@N-C	1166.2 (100), 1059.5 (200), 905.8 (500), 841.2 (800), 817.4 (1000), 724.8 (2000), 641.7 (5000), 593.2 (8000)	[11]
HBC-NiS/C	621 (200), 519 (500), 358 (1000), 170 (2000), 108 (3000)	[9]
NiS@NSC	601.2 (100), 530.4 (200), 491.5 (500), 479.1(1000),446.1(2000)	[10]
rGO@NiS	1025.7 (100), 933.6 (200), 835.8 (500), 752.1 (1000), 673.6 (2000), 538.1(5000)	[12]
NiS/C	827.8 (100), 715.0 (200), 551.8 (500), 455.6 (800), 384.5 (1000)	[13]
NiS⊂pCW⊂GN	625 (200),542 (500), 519 (800), 506 (1000), 476 (2000), 430(5000),374(10000)	[14]
NiS-GNS-CNT	935 (250),752 (500), 650 (1000), 565 (2000), 440 (4000), 330(8000)	[15]
Ni ₃ S ₂ /C	1370 (50), 1117 (100), 1035 (200), 891 (500), 787 (750), 717 (1000), 565 (2000)	This work

Table S2. Comparisons of the rate performance of Ni_xS_y -based anodes for LIBs.

Anodes	$D_{Li} ({ m cm}^2{ m s}^{-1})$	Methods	Ref.
NiS/C	$1.3 imes 10^{-10}$	CV	[13]
FeP@C	$1.04 imes10^{-14}$	CV	[16]
Ni-FeP@C	2.53×10^{-14}	CV	[10]
MoS_2	3.04×10^{-14}	EIS	[17]
Ni ₃ S ₂ -NCNFs	$2.47 imes10^{-7}$	CV	[18]
ZnSe/C	$2.48\times10^{\text{-12}}$	EIS	[19]
CoSe@C	$6.0 imes 10^{-11}$	EIS	[20]
SnSe/CoSe@C	3.6×10^{-9}	EIS	[20]
rGO/MnFe ₂ O ₄	$1.62 imes 10^{-6}$	CV	[21]
MnO ₂ @PNC	1.0×10 ⁻⁸	GITT	[22]
Co ₂ GeO ₄	6.3×10 ⁻⁸	CV	[23]
$Co_xO_y@PC$	6.6×10^{-17}	CV	[24]
Ov-MnO/Ni OCNs	8.43×10^{-12}	GITT	[25]
CFO@N-C	2.76×10^{-13}	EIS	[26]
O _v -MnO/Co NCPs	3.92×10^{-12}	EIS	[27]
Sb/Sb ₂ O ₃ -NC-450	$9.5384 imes 10^{-7}$	CV	[28]
Co-MnO@C-CNTs	$6.93 imes 10^{-14}$	GITT	[29]
MnO–CNTs@TiO2–C	$7.78 imes10^{-10}$	EIS	[30]
Mn ₂ Mo ₃ O ₈ @C	8.20×10^{-17}	EIS	[31]
F-GeO ₂ @C	F-GeO ₂ @C $2.8 \sim 5.7 \times 10^{-11}$ (discharge) $0.5 \sim 8.0 \times 10^{-11}$ (charge)		[32]
Ni ₃ S ₂ /C	2.71 × 10 ⁻⁹ (discharge) 2.27 × 10 ⁻⁹ (charge)	GITT	This work

Table S3. Comparisons of the lithium-ion diffusion rate of MC/Cs anode in LIBs.

References

- [1] H. Geng, S. F. Kong, Y. Wang, J. Mater. Chem. A. 2014, 2, 15152.
- [2] D. Han, N. Xiao, B. Liu, G. Song, J. Ding, Mater. Lett. 2017, 196, 119.
- [3] Z. Wang, X. Li, Y. Yang, Y. Cui, H. Pan, Z. Wang, B. Chen, G. Qian, J. Mater. Chem. A. 2014, 2, 7912.
- [4] Y. J. Lee, T. H. Ha, G. B. Cho, K. W. Kim, J. H. Ahn, K. K. Cho, J. Nanosci. Nanotechnol. 2020, 20, 6782.
- [5] G. Xia, X. Li, J. He, Y. Wang, Y. Gu, L. Liu, J. Huang, P. Dong, J. Duan, D. Wang, Y. Zhang, Y. Zhang, *Ceram. Int.* 2021, 47, 20948.
- [6] Q. Pan, J. Xie, S. Liu, G. Cao, T. Zhu, X. Zhao, *RSC Adv.* 2013, *3*, 3899.
- [7] N. Tronganh, Y. Gao, W. Jiang, H. Tao, S. Wang, B. Zhao, Y. Jiang, Z. Chen, Z. Jiao, *Appl. Surf. Sci.* 2018, 439, 386.
- [8] Z. Zhang, H. Zhao, Z. Zeng, C. Gao, J. Wang, Q. Xia, *Electrochim. Acta.* 2015, 155, 85.
- [9] J. Huang, G. Xia, L. Cheng, L. Liu, Y. Zhang, J. Duan, Y. Zhang, D. Wang, J. Electrochem. Soc. 2022, 169, 090511.
- [10] X. Dong, Z. P. Deng, L. H. Huo, X. F. Zhang, S. Gao, J. Alloy. Compd. 2019, 788, 984.
- [11] L. Li, D. Wang, S. Pei, R. Cao, X. Guo, J. Liu, Z. Zhang, Z. Zhou, G. Li, Appl. Surf. Sci. 2022, 605, 154782.
- [12] H. Ren, J. Wang, Y. Cao, W. Luo, Y. Sun, *Mater. Res. Bull.* 2021, 133, 111047.
- [13] L. Wang, Z. Wang, L. Xie, L. Zhu, X. Cao, *Electrochim. Acta.* 2020, 343, 136138.
- [14] C. Wu, J. Maier, Y. Yu, Adv. Mater. 2016, 28, 174.
- [15] X. Wang, X. Liu, G. Wang, Y. Zhou, H. Wang, J. Power Sources. 2017, 342, 105.
- [16] Z. Yan, Z. Sun, K. Yue, A. Li, H. Liu, Z. Guo, L. Qian, *Appl. Surf. Sci.* 2021, 554.
- [17] L. H. Wang, L. L. Ren, Y. F. Qin, Q. Li, Front. Chem. 2022, 9, 812247.
- [18] M. Guan, Z. Li, J. Ouyang, G. Li, L. Chen, M. Zhou, B. He, W. Xu, W. Wang,

Z. Hou, Mater. Today Commun. 2022, 31, 103652.

- [19] J. Yuan, X. Li, H. Li, W. Lai, Y. Gan, J. Yang, X. Zhang, J. Liu, X. Zhu, X. Li, *Chem.-Eur. J.* 2021, 27, 14989.
- [20] S. Lu, W. Luo, Z. Chao, Y. Liu, Z. Zhang, J. Fan, *Energy Fuels.* 2022, 36, 2260.
- [21] T. R. Madhura, P. Viswanathan, G. G. Kumar, R. Ramaraj, J. Electroanal. Chem. 2017, 792, 15.
- [22] X. Yuan, Z. Ma, S. Jian, H. Ma, Y. Lai, S. Deng, X. Tian, C. P. Wong, F. Xia, Y. Dong, *Nano Energy*. 2022, 97, 107235.
- [23] S. Yuvaraj, M. S. Park, V. G. Kumar, Y. S. Lee, D. W. Kim, J. Electrochem. Sci. Technol. 2017, 8, 323.
- [24] R. Tong, Y. Yan, X. Lu, Y. Li, Q. Tian, L. Yang, Z. Sui, J. Chen, J. Alloy. Compd. 2022, 899, 163293.
- [25] J. Lin, Y. Peng, R. C. K. Reddy, A. Zeb, X. Lin, Y. H. Sun, *Carbon Energy*.
 2022, 5, e226.
- [26] D. Dong, W. Zhang, W. Gong, X. Yu, X. Zuo, C. Wu, J. Alloy. Compd. 2021, 862, 158044.
- [27] J. Lin, C. Zeng, X. Lin, C. Xu, X. Xu, Y. Luo, ACS Nano. 2021, 15, 4594.
- [28] Z. Wang, F. Zeng, D. Zhang, X. Wang, W. Yang, Y. Cheng, C. Li, L. Wang, *Electrochim. Acta.* 2021, 395, 139210.
- [29] Q. Sun, Z. Cao, J. Zhang, H. Cheng, J. Zhang, Q. Li, H. Ming, G. Liu, J. Ming, *Adv. Funct. Mater.* 2021, 31, 2009122.
- [30] Q. Li, Y. Wu, Z. Wang, H. Ming, W. Wang, D. Yin, L. Wang, H. N. Alshareef, J. Ming, ACS Appl. Mater. Interfaces. 2020, 12, 16276.
- [31] Q. Sun, L. Sun, H. Ming, L. Zhou, H. Xue, Y. Wu, L. Wang, J. Ming, Nanoscale. 2020, 12, 4366.
- [32] Y. Lin, K. Zhong, J. Zheng, M. Liang, G. Xu, Q. Feng, J. Li, Z. Huang, ACS Appl. Energ. Mater. 2021, 4, 9848.