

## Supporting Information

# Niobium Sulfide Nanocomposite as Cathode Materials for All-Solid-State Lithium Batteries with Enhanced Electrochemical Performances

*Na Wang<sup>a,b</sup>, Mingyuan Chang<sup>b</sup>, Wenrui Xie<sup>a,b</sup>, Gaozhan Liu<sup>b</sup>, Lu Zhang<sup>b</sup>, Hao He<sup>a\*</sup>,*

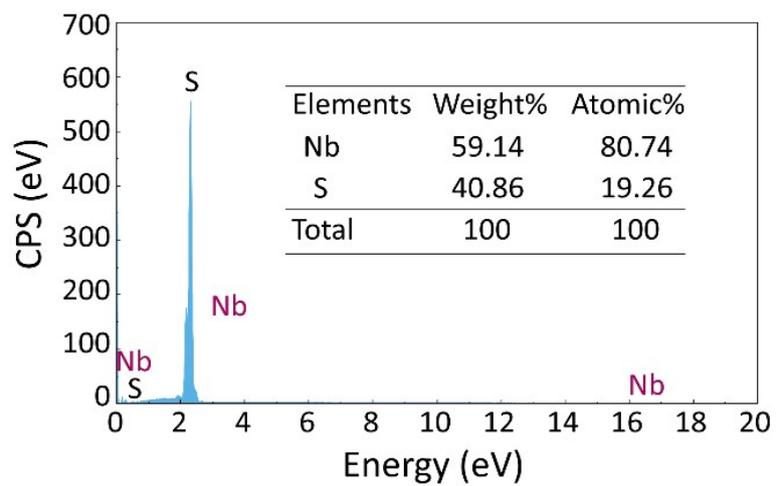
*Xiayin Yao<sup>b,c\*</sup>*

*<sup>a</sup> Key Laboratory of Materials Physics of Ministry of Education, School of Physics  
and Laboratory of Zhongyuan Light, Zhengzhou University, Zhengzhou, Henan  
450001, P. R. China*

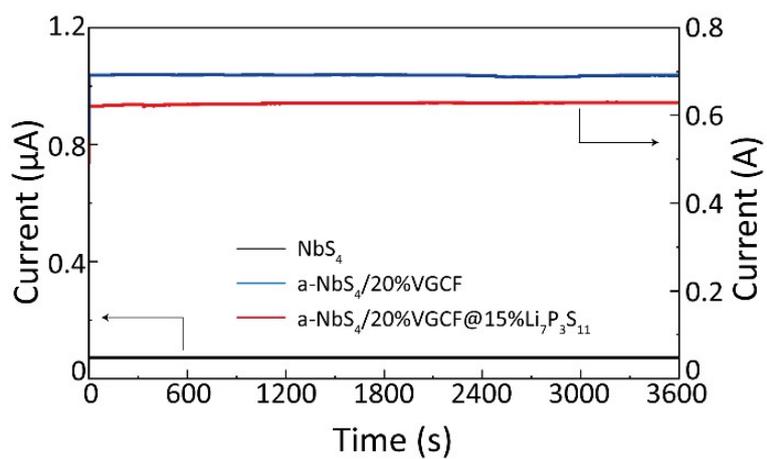
*<sup>b</sup> Ningbo Institute of Materials Technology and Engineering, Chinese Academy of  
Sciences, Ningbo 315201, P. R. China*

*<sup>c</sup> Center of Materials Science and Optoelectronics Engineering, University of Chinese  
Academy of Sciences, Beijing 100049, P. R. China.*

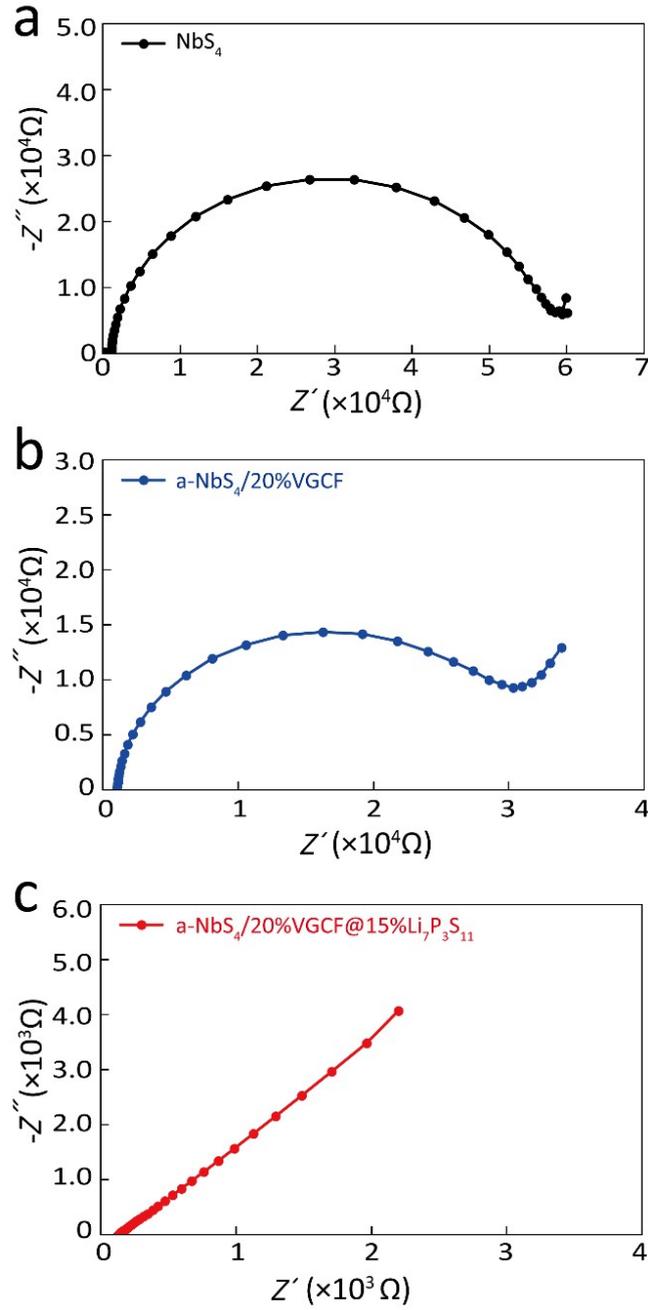
*\* Authors to whom correspondence should be addressed: yaoxy@nimte.ac.cn;  
hehao@zzu.edu.cn.*



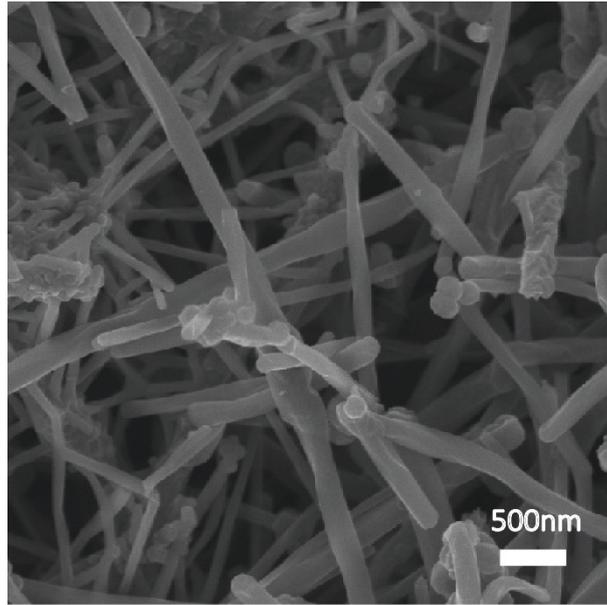
**Figure S1.** The EDS analysis in SEM and the composition results of NbS<sub>4</sub>.



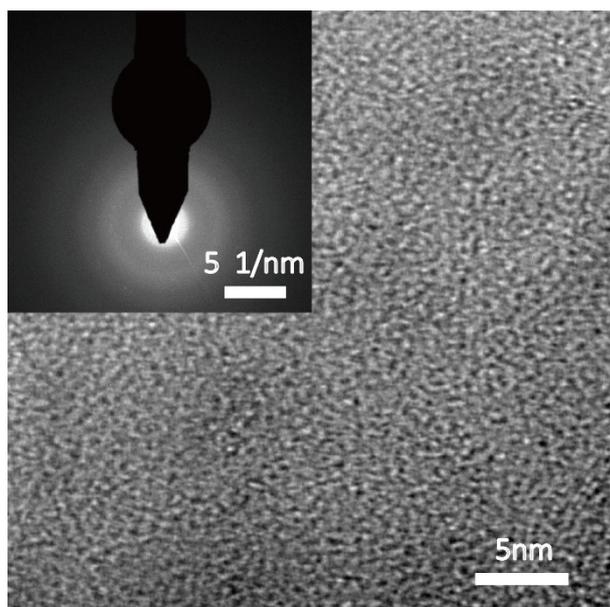
**Figure S2.** Current-time curves C/ $\text{NbS}_4$ /C, C/ $\text{a-NbS}_4/20\%\text{VGCF}$ /C and C/ $\text{a-NbS}_4/20\%\text{VGCF}@15\%\text{Li}_7\text{P}_3\text{S}_{11}$ /C cells under direct current polarization.



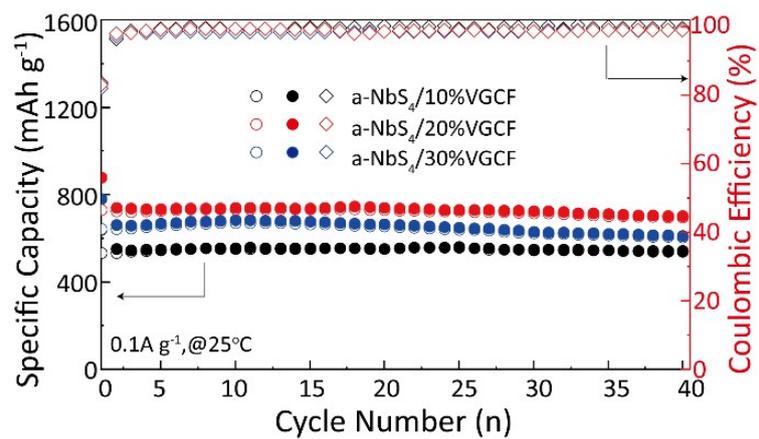
**Figure S3.** Impedance spectra of the (a)  $\text{Li}_{10}\text{GeP}_2\text{S}_{12}/\text{NbS}_4/\text{Li}_{10}\text{GeP}_2\text{S}_{12}$ , (b)  $\text{Li}_{10}\text{GeP}_2\text{S}_{12}/\text{a-NbS}_4/20\%\text{VGCF}/\text{Li}_{10}\text{GeP}_2\text{S}_{12}$  and (c)  $\text{Li}_{10}\text{GeP}_2\text{S}_{12}/\text{a-NbS}_4/20\%\text{VGCF}@15\%\text{Li}_7\text{P}_3\text{S}_{11}/\text{Li}_{10}\text{GeP}_2\text{S}_{12}$  cells.



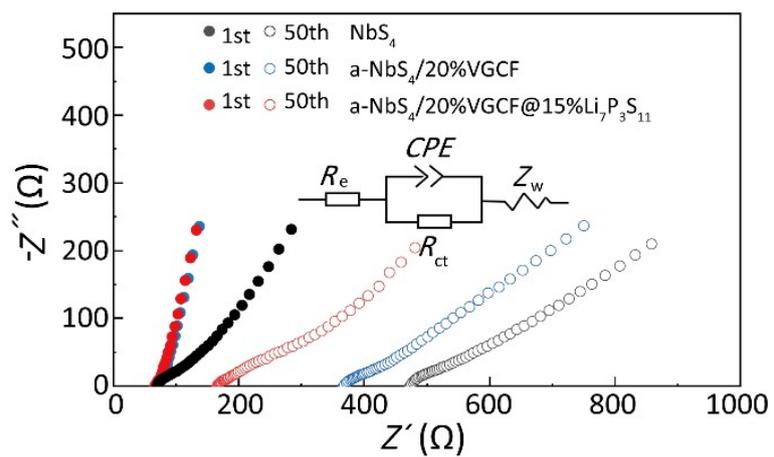
**Figure S4.** SEM image of VGCF.



**Figure S5.** HRTEM image and SAED pattern of a-NbS<sub>4</sub>/20%VGCF.



**Figure S6.** Cyclic performances of a-NbS<sub>4</sub>/10%VGCF, a-NbS<sub>4</sub>/20%VGCF and a-NbS<sub>4</sub>/30%VGCF cathodes at 0.1 A g<sup>-1</sup>.



**Figure S7.** Nyquist plots of  $\text{NbS}_4$ ,  $\text{a-NbS}_4/20\%\text{VGCF}$  and  $\text{a-NbS}_4/20\%\text{VGCF}@15\%\text{Li}_7\text{P}_3\text{S}_{11}$  electrodes cycled at  $0.1 \text{ A g}^{-1}$  after the 1st and 50th cycles. The inset is the equivalent circuit model.

**Table S1.** Comparison of energy densities of commercialized cathode materials with NbS<sub>4</sub>.

Material	Theoretical specific capacity (mAh g <sup>-1</sup> )	Actual specific capacity (mAh g <sup>-1</sup> )	Operating voltage (V)	Energy density (Wh Kg <sup>-1</sup> )	Ref.
4.5 V LiCoO <sub>2</sub>	274	190	4	760	[S1]
LiNi <sub>0.8</sub> Mn <sub>0.1</sub> Co <sub>0.1</sub> O <sub>2</sub>	273~285	210	3.7	777	[S1]
LiNi <sub>0.5</sub> Mn <sub>1.5</sub> O <sub>4</sub>	147	135	4.75	641	[S1]
Li-Rich 300	300~450	300	3.5	1050	[S1]
LiFePO <sub>4</sub>	170	165	3.45	569	[S2]
LiMn <sub>2</sub> O <sub>4</sub>	148	120	3.7	444	[S3]
NbS <sub>4</sub>	970	920.8	~1.8	~1630	This work

**Table S2.** The fitted results of EIS plots for NbS<sub>4</sub>, a-NbS<sub>4</sub>/20%VGCF and a-NbS<sub>4</sub>/20%VGCF@15%Li<sub>7</sub>P<sub>3</sub>S<sub>11</sub> cathodes after 1<sup>st</sup> and 50<sup>th</sup> cycles at 0.1 A g<sup>-1</sup>.

sample	after 1 <sup>st</sup> cycle		after 50 <sup>th</sup> cycle	
	$R_e$ ( $\Omega$ )	$R_{ct}$ ( $\Omega$ )	$R_e$ ( $\Omega$ )	$R_{ct}$ ( $\Omega$ )
NbS <sub>4</sub>	70.10	40.02	476.35	165.19
a-NbS <sub>4</sub> /20%VGCF	69.84	/	386.95	131.54
a-NbS <sub>4</sub> /20%VGCF@15%Li <sub>7</sub> P <sub>3</sub> S <sub>11</sub>	66.33	/	164.31	58.68

## References

- S1 W. Li, H. Xu, Q. Yang, J. Li, Z. Zhang, S. Wang, J. Peng, B. Zhang, X. Chen, Z. Zhang, M. Yang, Y. Zhao, Y. Geng, W. Huang, Z. Ding, L. Zhang, Q. Tian, H. Yu and H. Li, *Energy Storage Science and Technology*, 2020, **9**, 448-478.
- S2 Y. M. Zhu, Z. W. Ruan, S. Z. Tang and V. Thangadurai, *Ionics*, 2014, **20**, 1501-1510.
- S3 Z. I. Radzi, K. H. Arifin, M. Z. Kufian, V. Balakrishnan, S. R. S. Raihan, N. Abd Rahim and R. Subramaniam, *Journal of Electroanalytical Chemistry*, 2023, **928**, 1572-6657.