

## **Supplementary Information for**

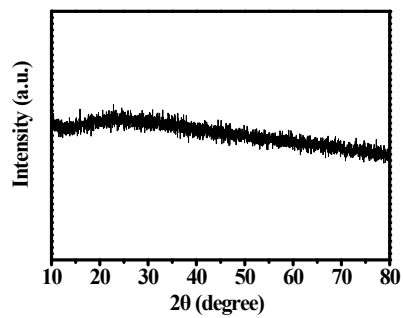
# **Boosting lithium-ion and sodium-ion storage performances of pyrite by regulating energy barrier of ion transport**

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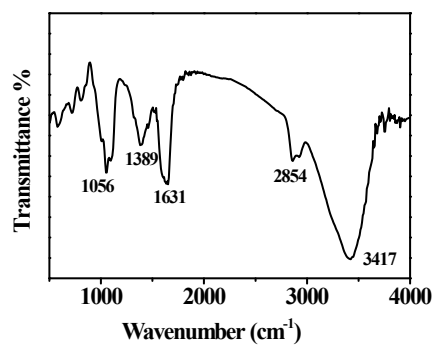
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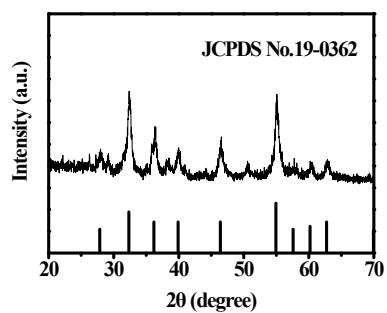
## Supplementary Figures



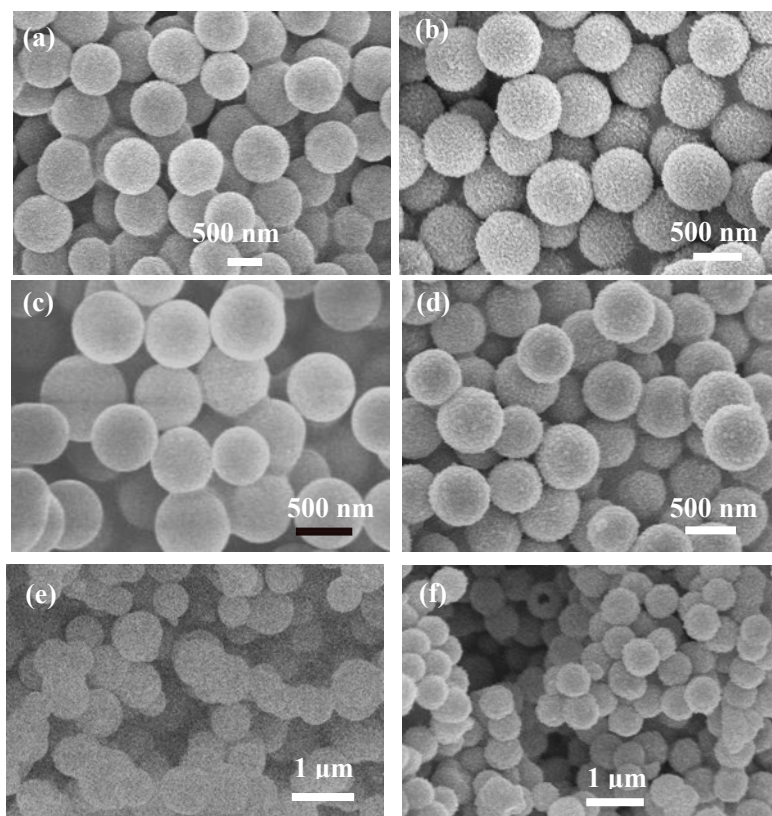
**Fig. S1** The XRD pattern of the FeCo-glycerate precursor.



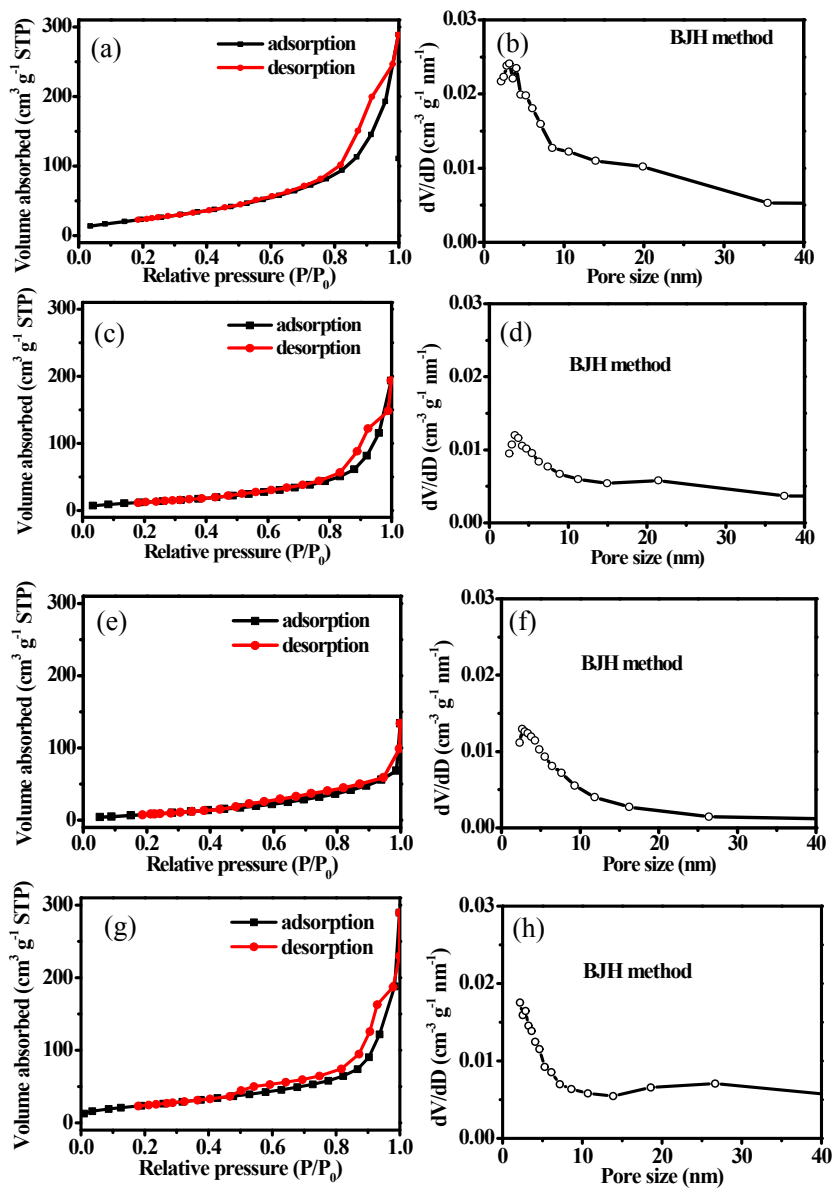
**Fig. S2** FTIR spectrum of the Fe<sub>0.3</sub>Co<sub>0.7</sub>S<sub>2</sub> precursor.



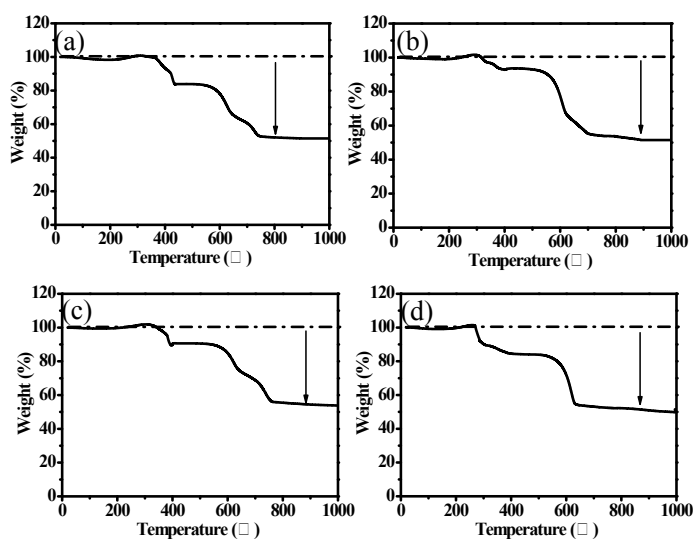
**Fig. S3** Powder XRD pattern of the as-prepared CoS<sub>2</sub> sample.



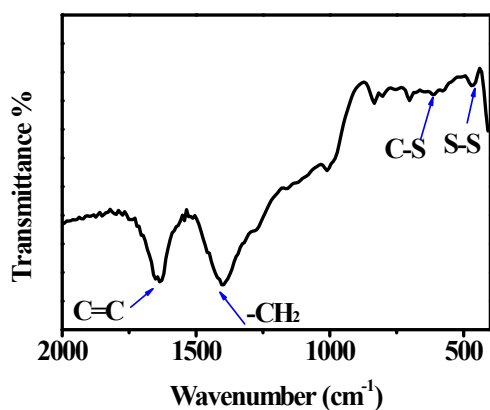
**Fig. S4** SEM images of (a)  $\text{FeS}_2$  precursor and (b)  $\text{FeS}_2$ , (c)  $\text{Fe}_{0.4}\text{Co}_{0.6}\text{S}_2$  precursor and (d)  $\text{Fe}_{0.4}\text{Co}_{0.6}\text{S}_2$ , (e)  $\text{Fe}_{0.8}\text{Co}_{0.2}\text{S}_2$  precursor and (f)  $\text{Fe}_{0.8}\text{Co}_{0.2}\text{S}_2$ .



**Fig. S5** N<sub>2</sub> adsorption-desorption isotherms and pore size distribution curves of (a,b) Fe<sub>0.7</sub>Co<sub>0.3</sub>S<sub>2</sub>, (c,d) Fe<sub>0.8</sub>Co<sub>0.2</sub>S<sub>2</sub>, (e,f) Fe<sub>0.4</sub>Co<sub>0.6</sub>S<sub>2</sub>, and (g,h) FeS<sub>2</sub>.

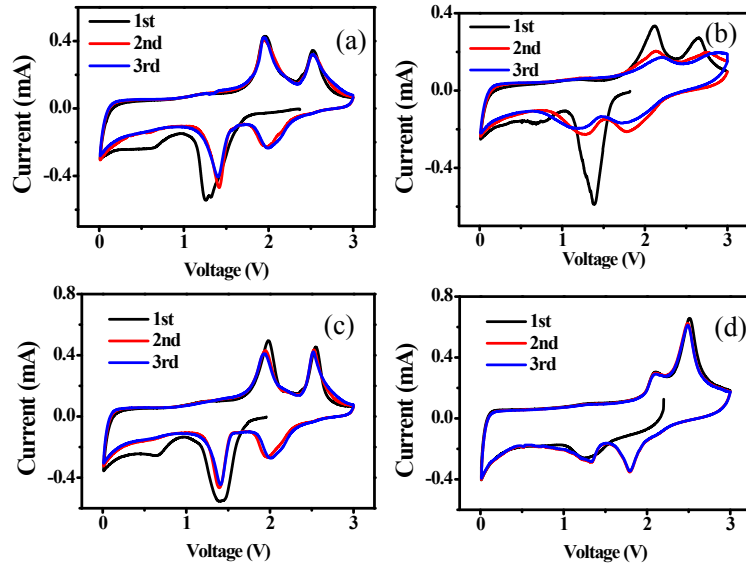


**Fig. S6** TGA curves of (a)  $\text{Fe}_{0.7}\text{Co}_{0.3}\text{S}_2$  (b)  $\text{Fe}_{0.8}\text{Co}_{0.2}\text{S}_2$  (c)  $\text{Fe}_{0.6}\text{Co}_{0.4}\text{S}_2$  (d)  $\text{FeS}_2$ . The carbon content is about 23.5 wt%

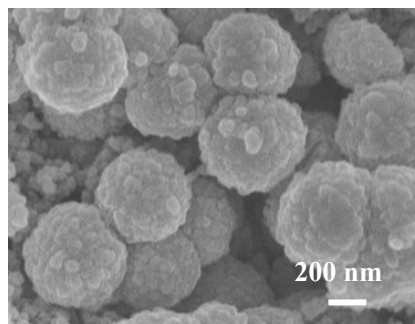


**Fig. S7** FTIR spectrum of  $\text{Fe}_{0.7}\text{Co}_{0.3}\text{S}_2$ .

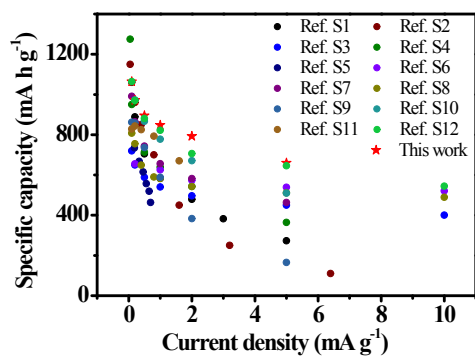
FTIR spectrum was used to identify the surface functional groups of  $\text{Fe}_{0.7}\text{Co}_{0.3}\text{S}_2$ . The peaks at 1636, 1396, 619 and 471  $\text{cm}^{-1}$  can be assigned to C=C, -CH<sub>2</sub>, C-S and S-S stretching vibrations, respectively.



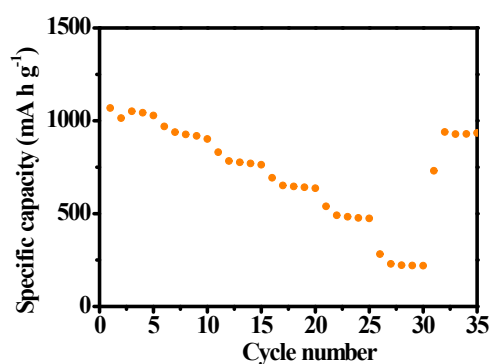
**Fig. S8** CV curves of (a)  $\text{Fe}_{0.8}\text{Co}_{0.2}\text{S}_2$ , (b)  $\text{Fe}_{0.4}\text{Co}_{0.6}\text{S}_2$ , (c)  $\text{FeS}_2$ , and (d)  $\text{CoS}_2$ .



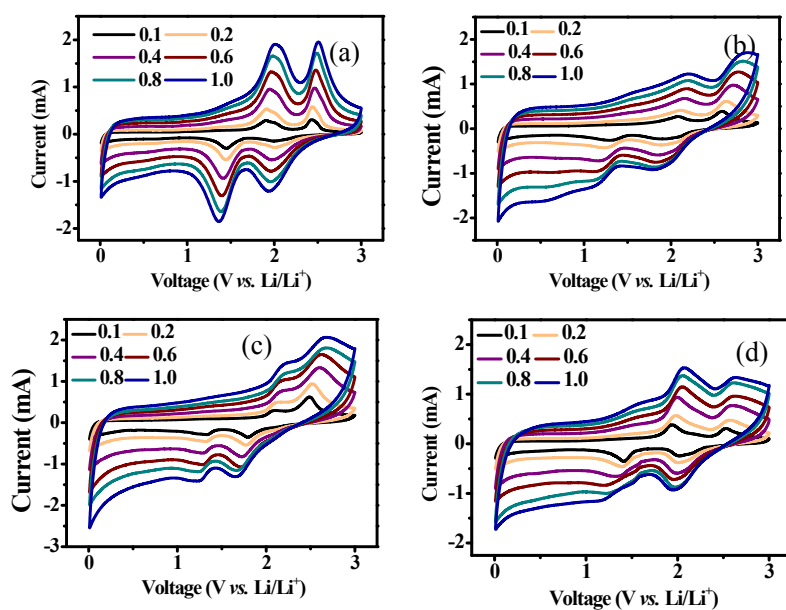
**Fig. S9** The *ex*-SEM image of  $\text{Fe}_{0.7}\text{Co}_{0.3}\text{S}_2$  after 100 cycles in LIBs.



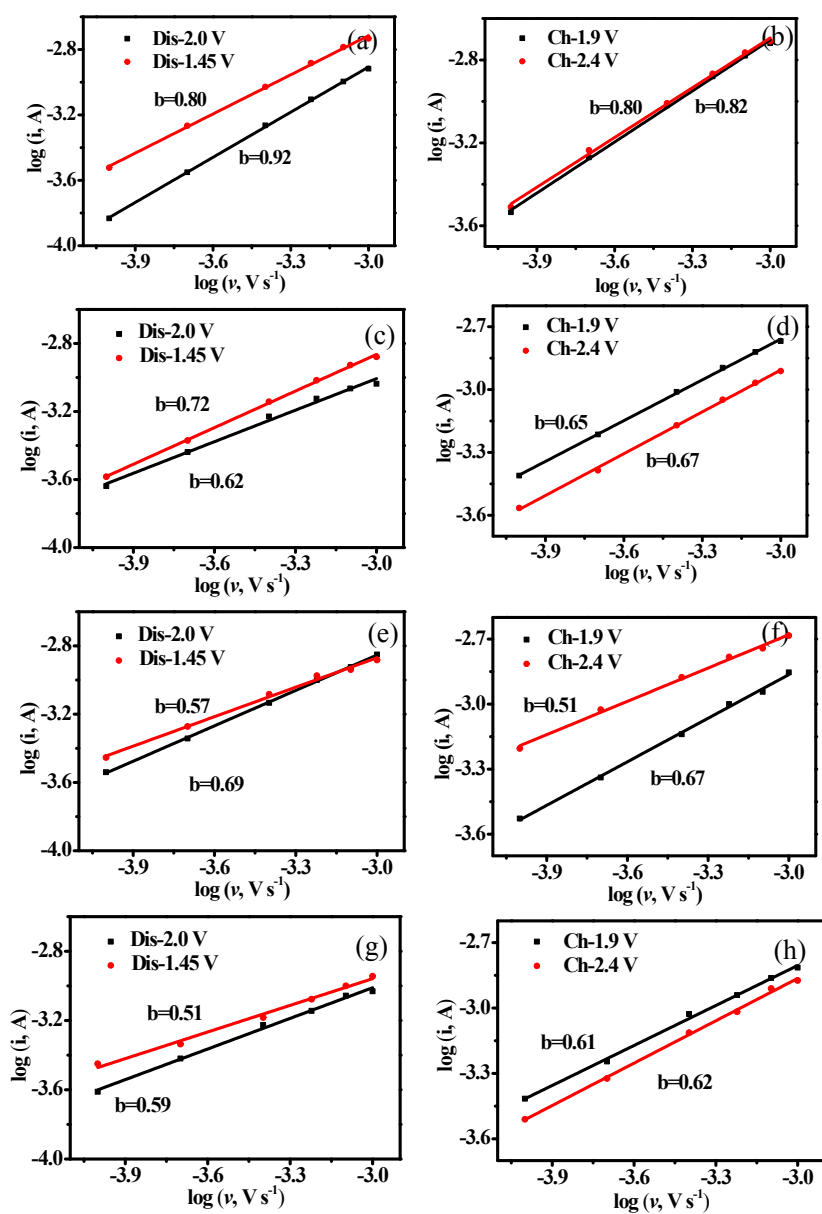
**Fig. S10** Comparison of Fe<sub>0.7</sub>Co<sub>0.3</sub>S<sub>2</sub> electrode with FeS<sub>2</sub>-based electrodes reported in the literatures for LIBs.



**Fig. S11** Rate performance of CoS<sub>2</sub> at 0.1, 0.2, 0.5, 1, 2 and 5 A g<sup>-1</sup>.

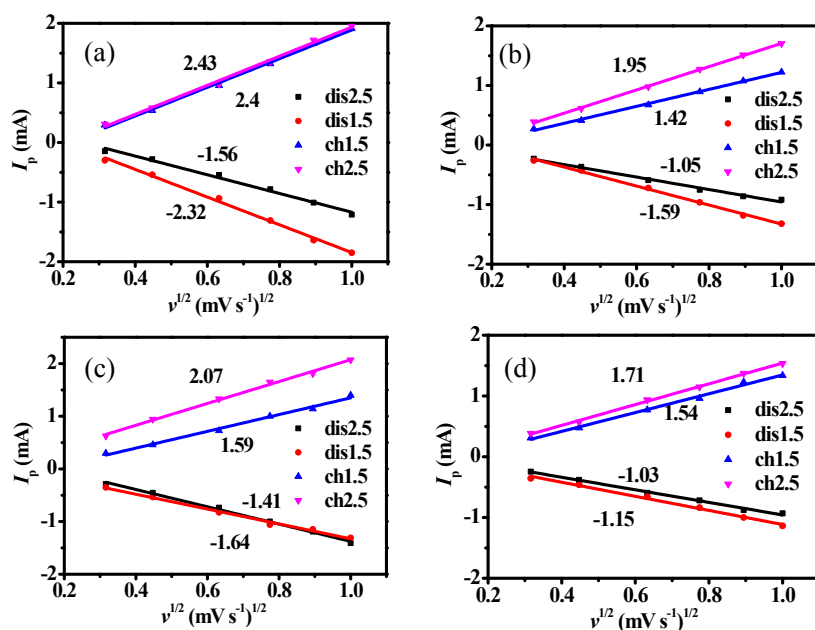


**Fig. S12** CV curves of (a) Fe<sub>0.7</sub>Co<sub>0.3</sub>S<sub>2</sub>, (b) Fe<sub>0.8</sub>Co<sub>0.2</sub>S<sub>2</sub>, (c) Fe<sub>0.4</sub>Co<sub>0.6</sub>S<sub>2</sub>, and (d) FeS<sub>2</sub> at different scan rates.

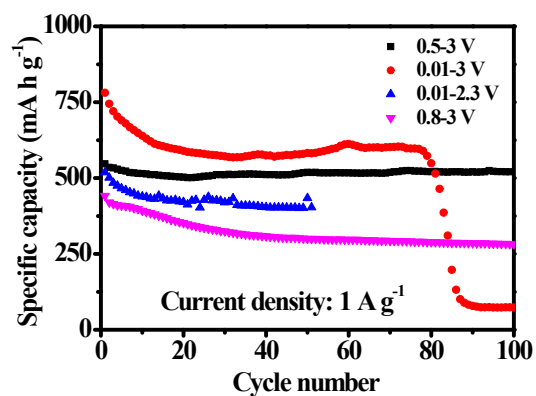


**Fig. S13** Log(*i*) vs. log(*v*) plots at each redox peaks of the as-prepared (a,b) Fe<sub>0.7</sub>Co<sub>0.3</sub>S<sub>2</sub>, (c,d) Fe<sub>0.8</sub>Co<sub>0.2</sub>S<sub>2</sub>, (e,f) Fe<sub>0.4</sub>Co<sub>0.6</sub>S<sub>2</sub>, and (g,h) FeS<sub>2</sub> samples.

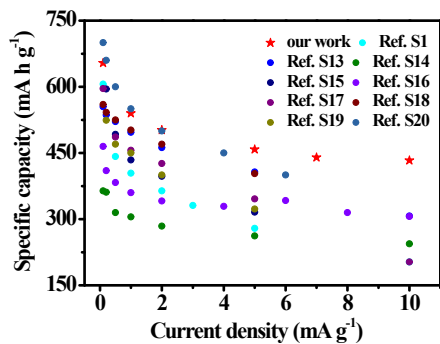




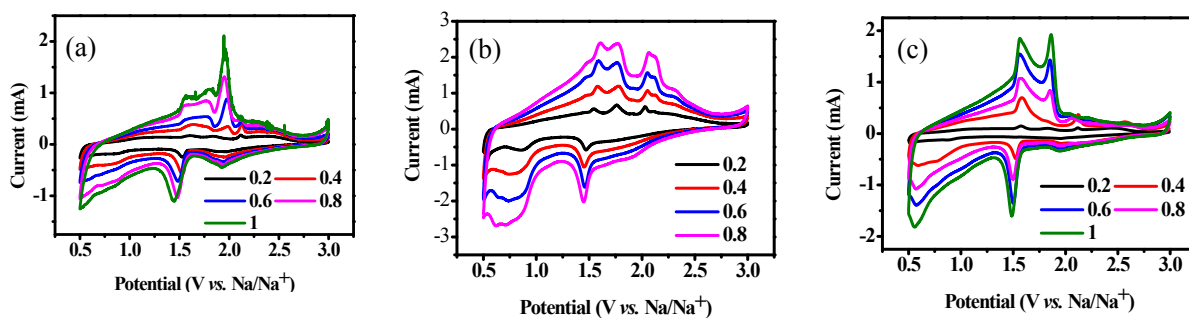
**Fig. S14**  $I_p$  vs.  $v^{1/2}$  plots at each redox peaks of the as-prepared (a)  $\text{Fe}_{0.7}\text{Co}_{0.3}\text{S}_2$ , (b)  $\text{Fe}_{0.8}\text{Co}_{0.2}\text{S}_2$ , (c)  $\text{Fe}_{0.4}\text{Co}_{0.6}\text{S}_2$ , and (d)  $\text{FeS}_2$  samples.



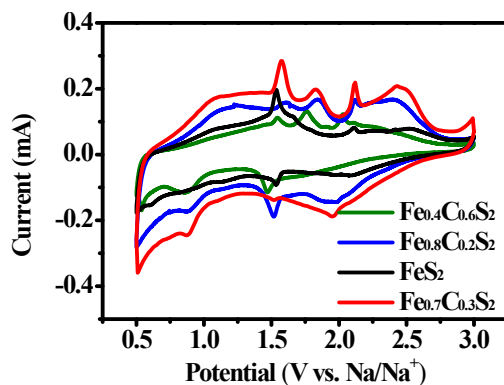
**Fig. S15** Cycling performances of  $\text{Fe}_{0.7}\text{Co}_{0.3}\text{S}_2$  at a current density of  $1 \text{ A g}^{-1}$  with different potential ranges.



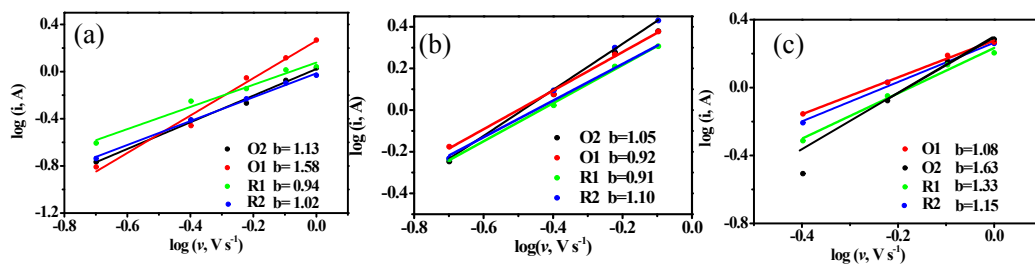
**Fig. S16** Comparison of high-rate performance of  $\text{Fe}_{0.7}\text{Co}_{0.3}\text{S}_2$  electrode with  $\text{FeS}_2$ -based electrodes reported in the literatures for SIBs.



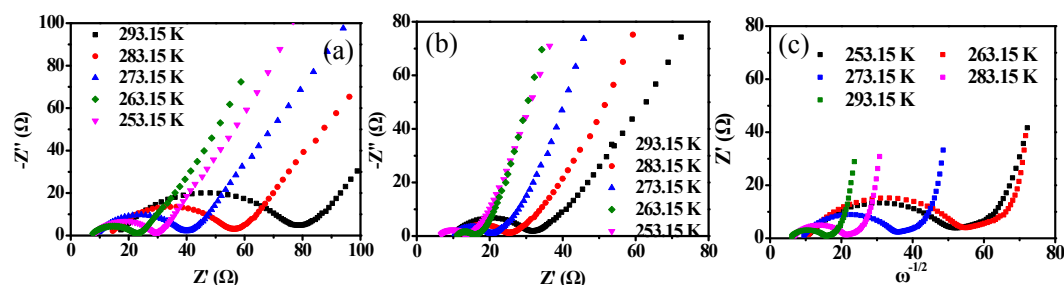
**Fig. S17** CV curves of (a)  $\text{Fe}_{0.8}\text{Co}_{0.2}\text{S}_2$  (b)  $\text{Fe}_{0.4}\text{Co}_{0.6}\text{S}_2$ , and (c)  $\text{FeS}_2$  at different scan rates.



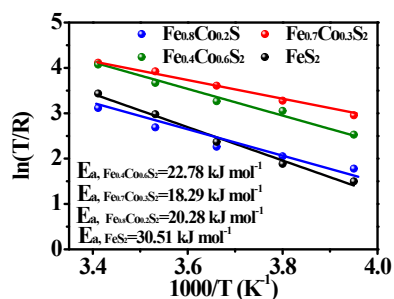
**Fig. S18** Typical CV curves of the as-prepared  $\text{Fe}_{0.7}\text{Co}_{0.3}\text{S}_2$ ,  $\text{Fe}_{0.8}\text{Co}_{0.2}\text{S}_2$ ,  $\text{Fe}_{0.4}\text{Co}_{0.6}\text{S}_2$  and  $\text{FeS}_2$  samples at the scan rate of 0.2  $\text{mV s}^{-1}$ .



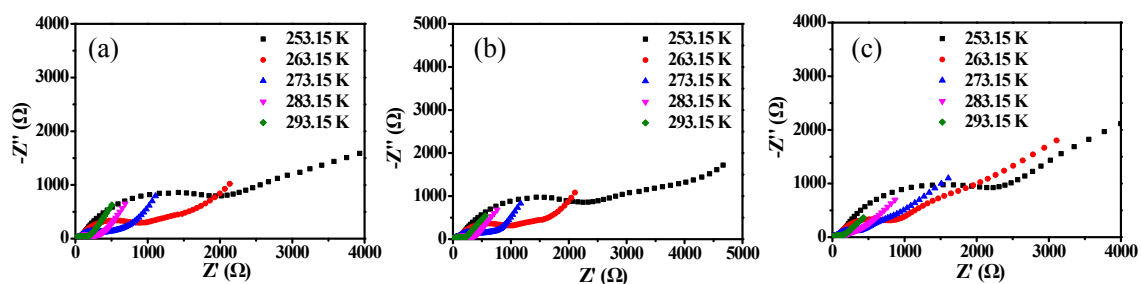
**Fig. S19** Log (i) vs Log (v) plots at each peaks of (a)  $Fe_{0.8}Co_{0.2}S_2$ , (b)  $Fe_{0.4}Co_{0.6}S_2$ , and (c)  $FeS_2$ .



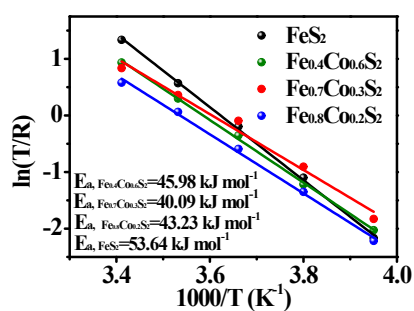
**Fig. S20** EIS plots of (a)  $Fe_{0.8}Co_{0.2}S_2$ , (b)  $Fe_{0.4}Co_{0.6}S_2$  and (c)  $FeS_2$  samples at different temperatures in SIBs.



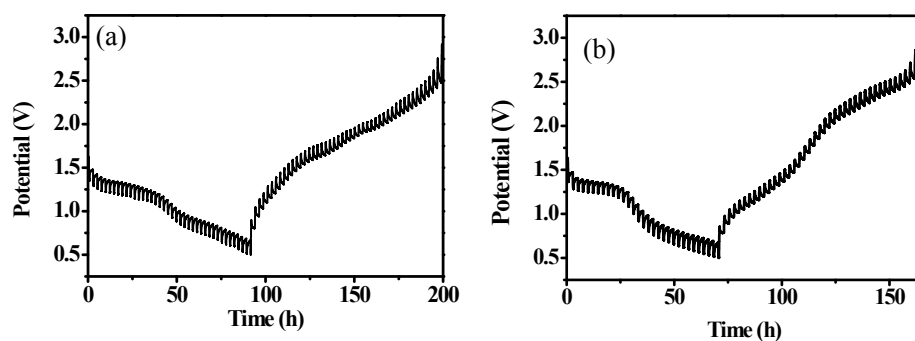
**Fig. S21** Arrhenius plots of  $\ln(T/R_{ct})$  versus  $1/T$  system of  $Fe_{0.8}Co_{0.2}S_2$ ,  $Fe_{0.7}Co_{0.3}S_2$ ,  $Fe_{0.4}Co_{0.6}S_2$ , and  $FeS_2$  in SIB (the inset displaying the  $E_a$  values).



**Fig. S22** EIS plots of (a)  $\text{Fe}_{0.4}\text{Co}_{0.6}\text{S}_2$ , (b)  $\text{Fe}_{0.8}\text{Co}_{0.2}\text{S}_2$  and (c)  $\text{FeS}_2$  samples at different temperatures in LIBs.



**Fig. S23** Arrhenius plots of  $\ln(T/R_{ct})$  versus  $1/T$  system of  $\text{Fe}_{0.8}\text{Co}_{0.2}\text{S}_2$ ,  $\text{Fe}_{0.7}\text{Co}_{0.3}\text{S}_2$ ,  $\text{Fe}_{0.4}\text{Co}_{0.6}\text{S}_2$ , and  $\text{FeS}_2$  in LIBs (the inset displaying the  $E_a$  values).



**Fig. S24** GITT profiles of (a)  $\text{Fe}_{0.7}\text{Co}_{0.3}\text{S}_2$  and (b)  $\text{FeS}_2$  in SIBs.

**Table S1.** ICP results of the Fe<sub>0.8</sub>Co<sub>0.2</sub>S<sub>2</sub>, Fe<sub>0.7</sub>Co<sub>0.3</sub>S<sub>2</sub>, Fe<sub>0.4</sub>Co<sub>0.6</sub>S<sub>2</sub>, and FeS<sub>2</sub> samples.

Element	Fe <sub>0.8</sub> Co <sub>0.2</sub> S <sub>2</sub>	Fe <sub>0.7</sub> Co <sub>0.3</sub> S <sub>2</sub>	Fe <sub>0.4</sub> Co <sub>0.6</sub> S <sub>2</sub>
	Atom (%)	Atom (%)	Atom (%)
Fe	79.8%	70.2%	39.6%
Co	20.2%	29.8%	60.4%

**Table S2.** The pseudocapacitive contributions of Fe<sub>0.7</sub>Co<sub>0.3</sub>S<sub>2</sub>, Fe<sub>0.8</sub>Co<sub>0.2</sub>S<sub>2</sub>, Fe<sub>0.7</sub>Co<sub>0.3</sub>S<sub>2</sub>, Fe<sub>0.4</sub>Co<sub>0.6</sub>S<sub>2</sub>, and FeS<sub>2</sub> samples.

Scan rate	Pseudocapacitive contribution				
	Fe <sub>0.8</sub> Co <sub>0.2</sub> S <sub>2</sub>	Fe <sub>0.7</sub> Co <sub>0.3</sub> S <sub>2</sub>	Fe <sub>0.4</sub> Co <sub>0.6</sub> S <sub>2</sub>	FeS <sub>2</sub>	CoS <sub>2</sub>
0.1	47%	80.8%	40%	44.5%	48.9%
0.2	52.8%	83.7%	43.75%	50.1%	56.6%
0.4	60.3%	87.7%	52.63%	56.3%	68.3%
0.6	66.4%	90%	57.28%	64.8%	74.5%
0.8	72.1%	92.4%	65.88%	68.4%	85.9%
1	78.2%	97.8%	68.46%	76.5%	89.3%

**Table S3.** The D values on the fitting slopes of I<sub>p</sub>/v<sup>1/2</sup> for all samples in LIBs.

Samples	D values (cm <sup>2</sup> s <sup>-1</sup> )				
	Dis2.5	Dis1.5	Ch2.5	Ch1.5	average
Fe <sub>0.7</sub> Co <sub>0.3</sub> S <sub>2</sub>	1.78*10 <sup>-12</sup>	3.93*10 <sup>-12</sup>	4.31*10 <sup>-12</sup>	4.21*10 <sup>-12</sup>	3.56*10 <sup>-12</sup>
Fe <sub>0.8</sub> Co <sub>0.2</sub> S <sub>2</sub>	8.05*10 <sup>-13</sup>	1.85*10 <sup>-12</sup>	2.78*10 <sup>-12</sup>	1.47*10 <sup>-12</sup>	1.63*10 <sup>-12</sup>
Fe <sub>0.4</sub> Co <sub>0.6</sub> S <sub>2</sub>	1.45*10 <sup>-12</sup>	1.96*10 <sup>-12</sup>	3.12*10 <sup>-12</sup>	1.85*10 <sup>-12</sup>	2.09*10 <sup>-12</sup>
FeS <sub>2</sub>	7.74*10 <sup>-13</sup>	9.66*10 <sup>-13</sup>	2.13*10 <sup>-12</sup>	1.73*10 <sup>-12</sup>	1.4*10 <sup>-12</sup>

## References

- S1 A. Huang, Q. Wang, Z. Ma, K. Rui, X. Huang, J. Zhu, W. Huang, *ACS Appl. Mater. Interfaces*, 2019, **11**, 39991.
- S2 P. Guo, H. Song, Y. Liu, and C. Wang, *ACS Appl. Mater. Interfaces*, 2017, **9**, 31752.
- S3 X. Xu, J. Liu, Z. Liu, J. Shen, R. Hu, J. Liu, L. Ouyang, L. Zhang, *ACS Nano*, 2017, **11**, 9033.
- S4 R. Tan, J. Yang, J. Hu, K. Wang, Y. Zhao and F. Pan, *Chem. Commun.*, 2016, **52**, 986.
- S5 G. X. Pan, F. Cao, X. H. Xia, Y. J. Zhang, *J. Power Sources*, 2016, **332**, 383.
- S6 F. Zhang, C. Wang, G. Huang, D. Yin, L. Wang, *J. Power Sources*, 2016, **328** 56.
- S7 Z. Qiu, Y. Lin, H. Xin, P. Han, D. Li, B. Yang, P. Li, S. Ullah, H. Fan, C. Zhu, J. Xu, *Carbon*, 2018, **126**, 85.
- S8 Kun Wang, S. P. Huang, Y. Wu, N. N. Cai, N. Li, Q. Xiao and Z. Sun, *Nanoscale*, 2019, **11**, 16277.

- S9 S. Wang, P. Ning, S. Huang., W. Wang, S. Fei, Q. He, J. Zai, Y. Jiang, Z. Hu, X. Qian, Z. Chen, *J. Power Sources*, 2019, **436**, 226857.
- S10 X. Ding, C. Du, J. Li and X. Huang, *Sustain. Energ. Fuels*, 2019, **3**, 701.
- S11 . Zhang, G. Zhao, X. Lv, Y. Tian, L. Yang, G. Zou, H. Hou, H. Zhao, *ACS Appl. Mater. Interfaces*, 2019, **11**, 6154.
- S12 Q. T. Xu, J. C. Li, H. G. Xue, S. P. Guo, *J. Power Sources*, 2018, **396**, 675.
- S13 R. Zang, P. Li, X. Guo, Z. Man, S. Zhang, C. Wang and G. Wang, *J. Mater. Chem. A*, 2019, **7**, 14051.
- S14 L. Yao, B. Wang, Y. Yang, X. Chen, J. Hu, D. Yang and A. Dong, *Chem. Commun.*, 2019, **55**, 1229.
- S15 Z. Chen, S. Li, Y. Zhao, M. F. Aly Aboud, I. Shakir and Y. Xu, *J. Mater. Chem. A*, 2019, **7**, 26342.
- S16 Y. Zhao, J. Wang, C. Ma, Y. Li , J. Shi, Z. Shao, *Chem. Eng. J.*, 2019, **378**, 122168.
- S17 W. Zhao, C. Guo and C. M. Li, *J. Mater. Chem. A*, 2017, **5**, 19195.
- S18 Z. Liu, T. Lu, T. Song, X. Y. Yu, X. W. Lou and U. Paik, *Energy Environ. Sci.*, 2017, **10**, 1576.
- S19 K. Chen, W. Zhang, L. Xue, W. Chen, X. Xiang, M. Wan and Y. Huang, *ACS Appl. Mater. Interfaces*, 2017, **9**, 1536.
- S20 F. Wang, W. Zhang, H. Zhou, H. Chen, Z. Huang, Z. Yan, R. Jiang, C. Wang, Z. Tan, Y. Kuang, *Chem. Eng. J.*, 2020, **380**, 122549.