

Supplementary Information

TiS₂/Celgard separator as efficient polysulfide shuttling inhibitor for high performance lithium-sulfur batteries

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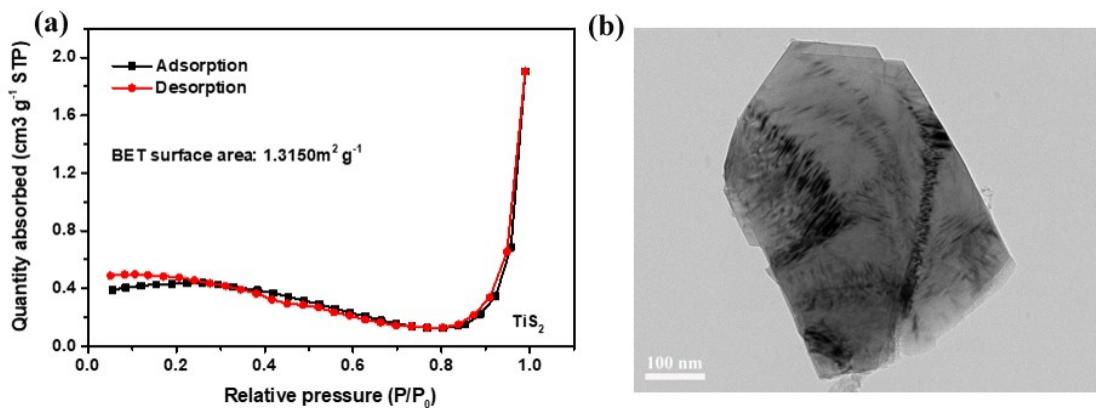


Fig. S1 (a) N₂ adsorption-desorption isotherms of TiS₂. (b) TEM images of TiS₂

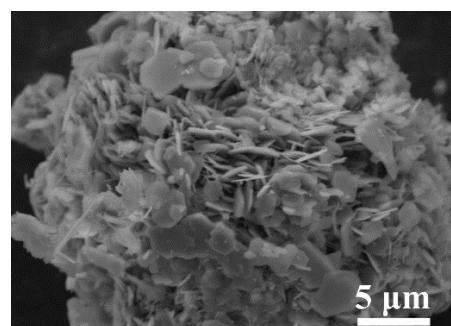


Fig. S2 The low-magnification SEM images of TiS₂

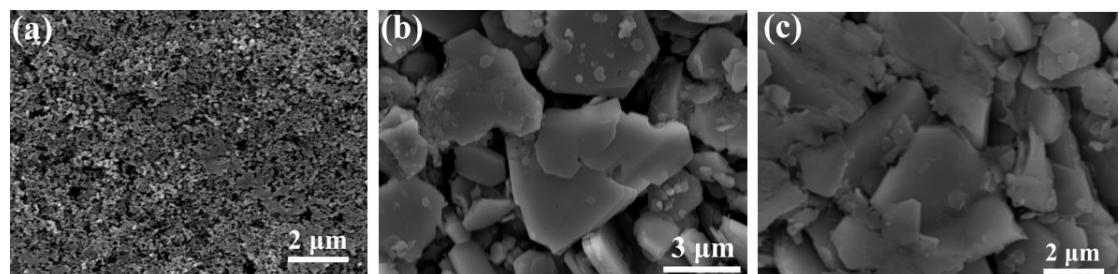


Fig. S3 SEM images of (a) Super P/Celgard, (b)TiS₂-SC/Celgard, and (c) TiS₂-VF/Celgard

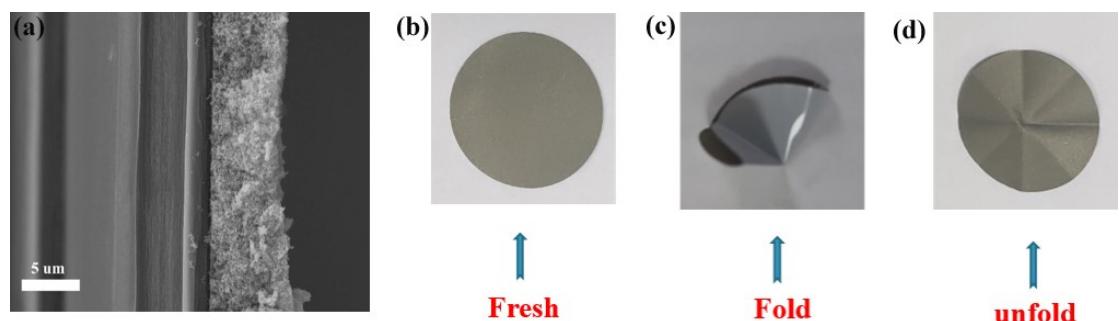


Fig. S4 (a) cross section of Super P layers. Photographs of as prepared TiS_2 -

VF/Celgard separator. Front side (b), folded (c) and unfolded (d).

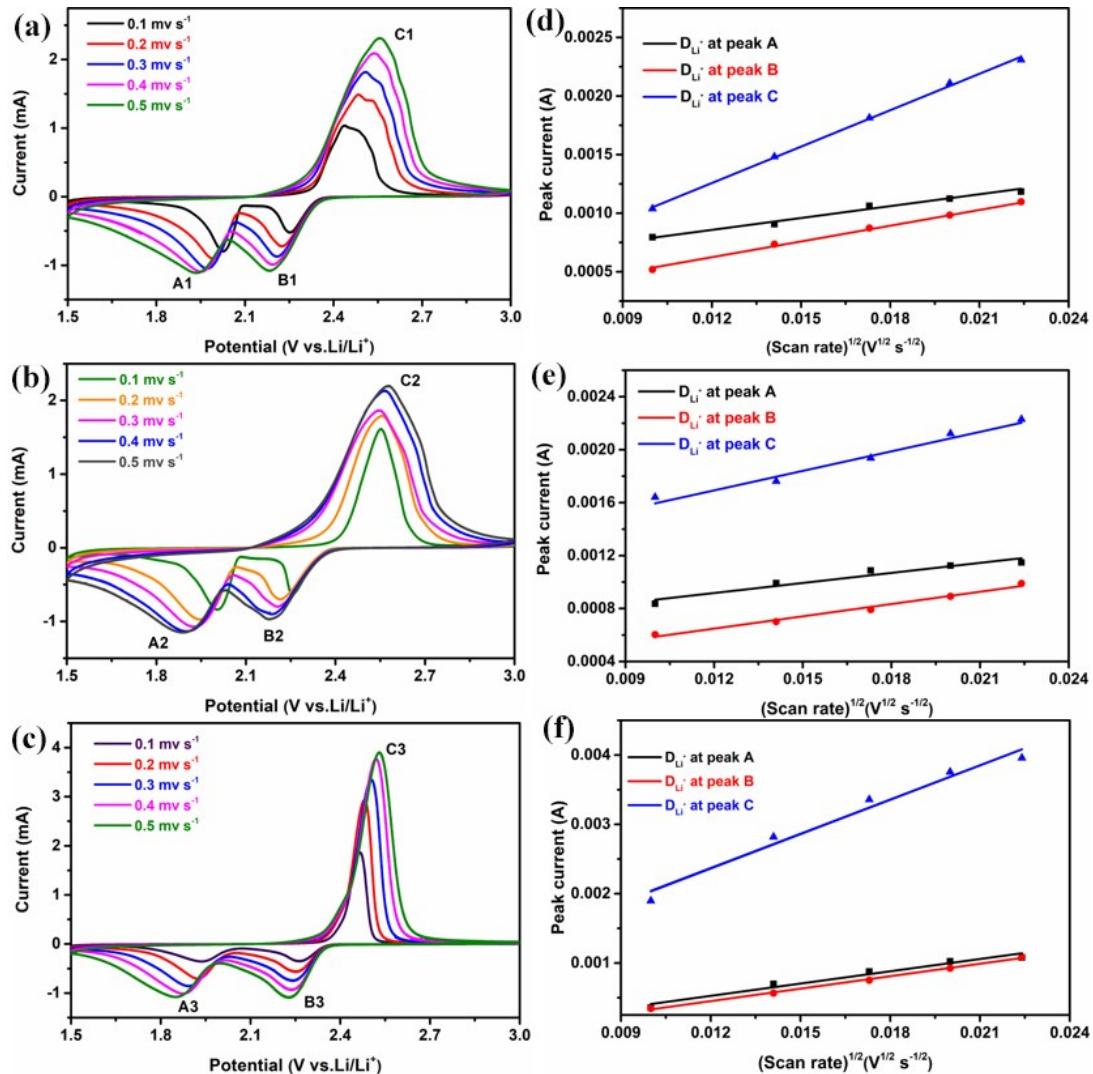


Fig. S5 (a-f) CV curves at various scan rates and corresponding linear fits of the peak

currents of the Li-S batteries with a, d) Celgard; b,e) Super P/Celgard; c,f) TiS_2 -

SC/Celgard.

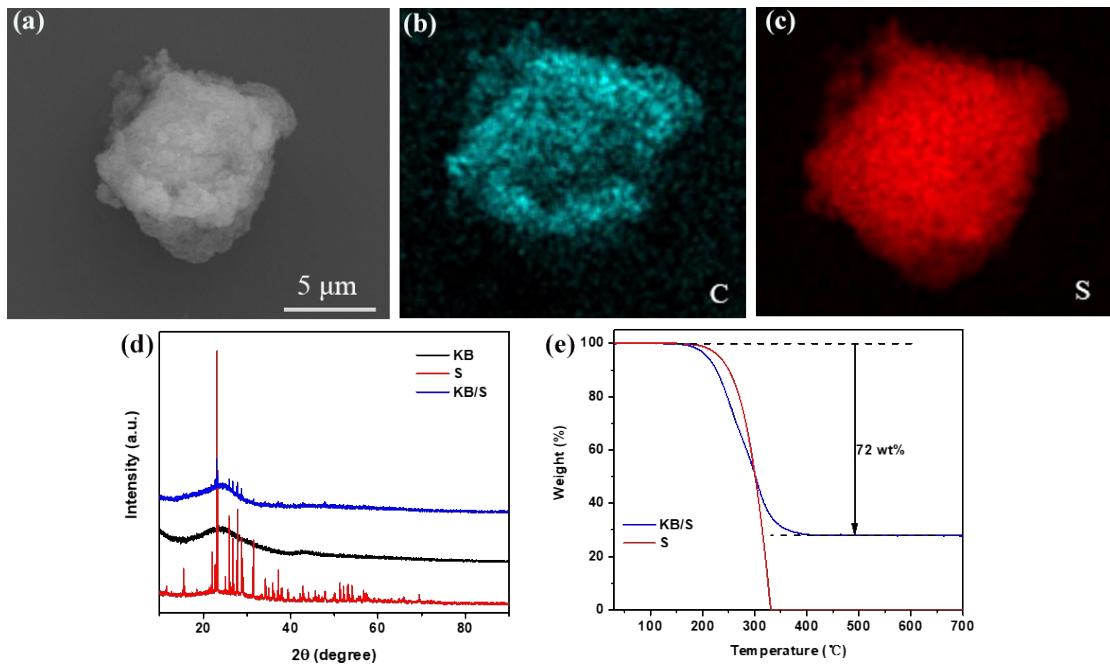


Fig. S6 (a) SEM and (b-c) elemental mapping images of KB/S; (d) XRD patterns for KB, S and KB/S; (e) TGA curve of the prepared S and KB/S composite under N₂ atmosphere.

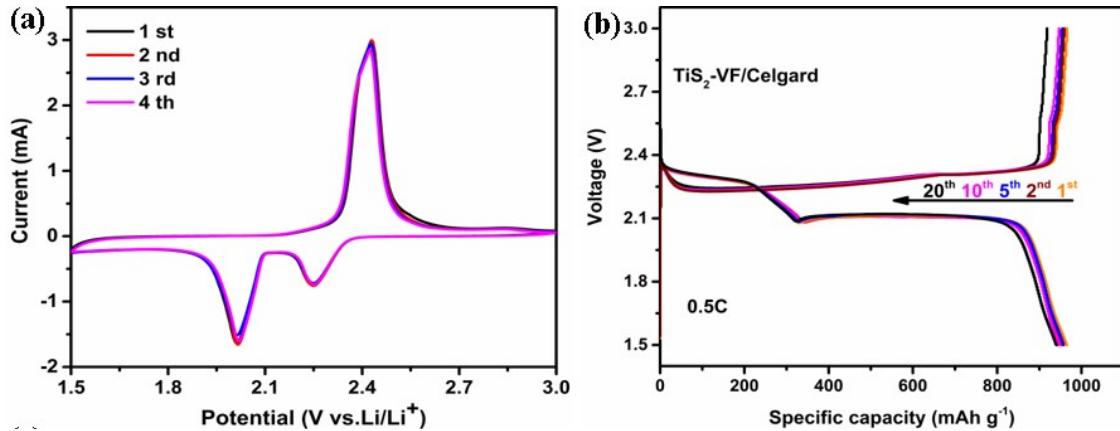


Fig. S7 Electrochemical performance of Li-S batteries with Celgard, Super P/Celgard, TiS₂-SC/Celgard and TiS₂-VF/Celgard separators: (a) Cyclic voltammogram profile for Li-S battery with TiS₂-VF/Celgard separator at scan rate of 0.2 mV s⁻¹. (b) Galvanostatic charge–discharge profiles at 0.5 C.

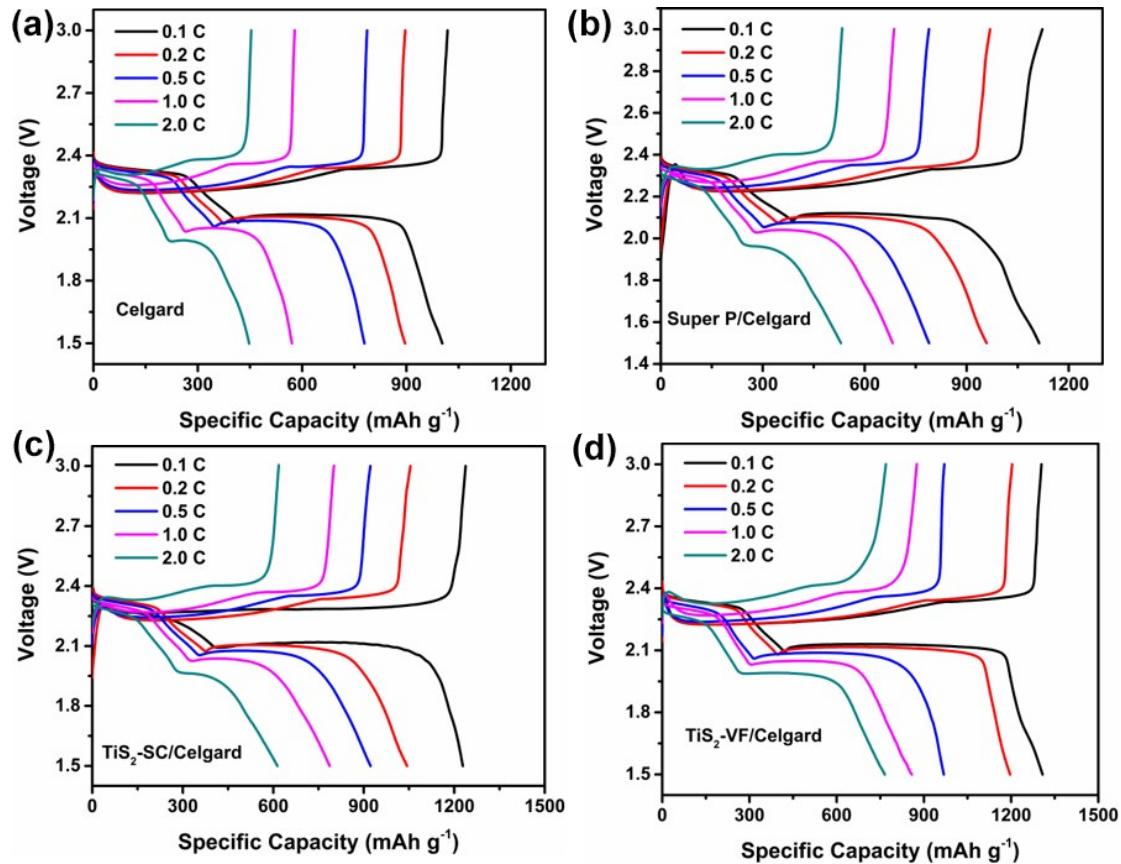


Fig. S8 Galvanostatic charge-discharge profiles of Li-S batteries with Celgard, Super P/Celgard, $\text{TiS}_2\text{-SC/Celgard}$ and $\text{TiS}_2\text{-VF/Celgard}$ separators at different rate.

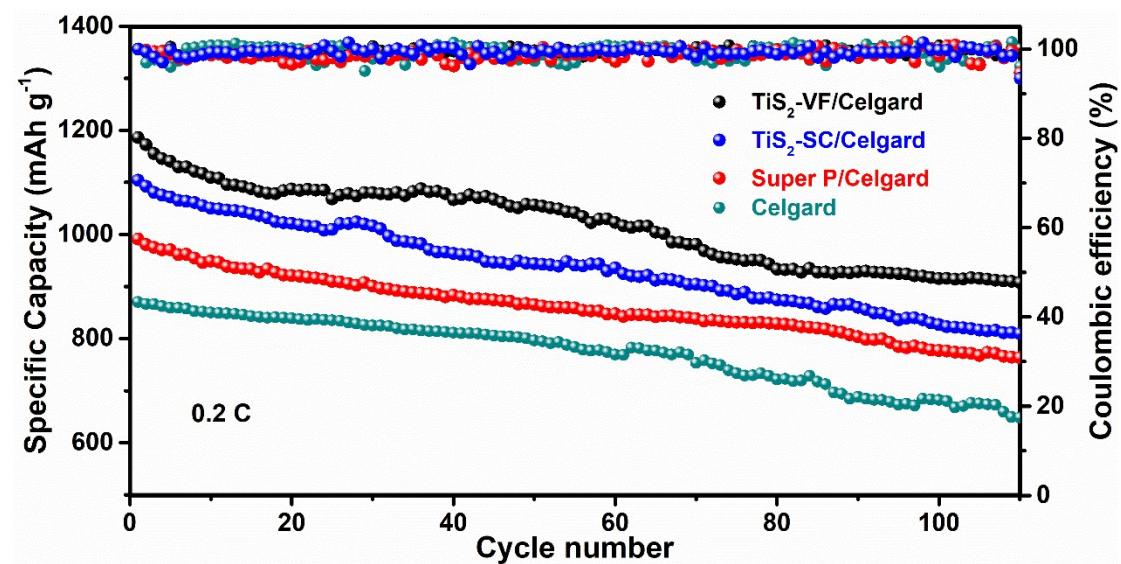


Fig. S9 Electrochemical performance of Li-S batteries with Celgard, Super P/Celgard, $\text{TiS}_2\text{-SC/Celgard}$ and $\text{TiS}_2\text{-VF/Celgard}$ separators: long-time cycling performance at 0.2 C.

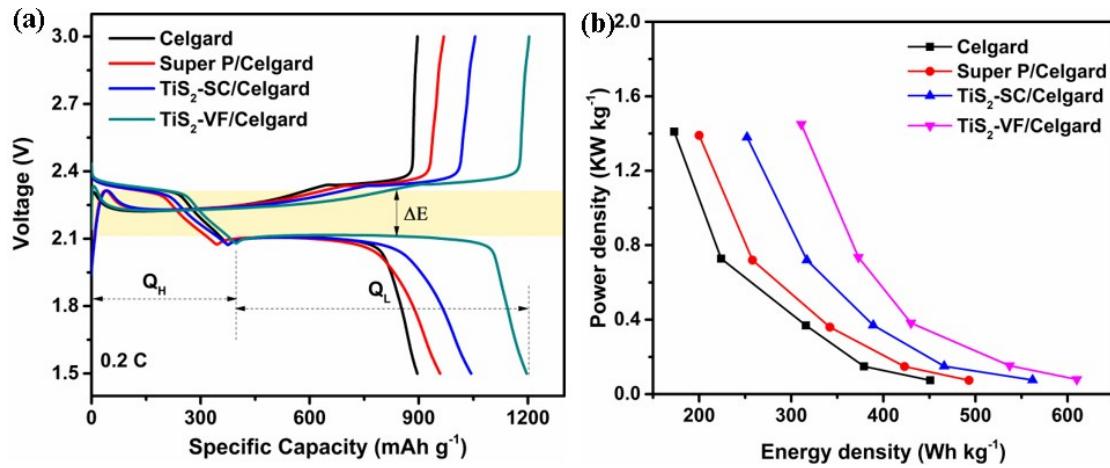


Fig. S10 (a) charge/discharge curves of Li-S batteries with Celgard, Super P/Celgard, TiS₂-SC/Celgard and TiS₂-VF/Celgard separators at 0.2 C; (b) Ragone plot. calculated from rate performances of Li-S batteries with Celgard, Super P/Celgard, TiS₂-SC/Celgard and TiS₂-VF/Celgard separators in Fig. 6c; The power and energy densities are calculated based on the total device mass.

Table S1. The specific data derived from simulation equivalent circuits diagram of the Li-S batteries with Celgard, Super P/Celgard, TiS₂-SC/Celgard and TiS₂-VF/Celgard separators.

Parameters	Celgard		Super P/Celgard		TiS ₂ -SC/Celgard		TiS ₂ -VF/Celgard	
	before	after	before	after	before	after	before	after
R ₀ (Ω)	6.55	10.87	7.14	13.96	18.62	4.39	3.675	7.77
R _{ct} (Ω)	110.25	38.37	117.66	31.64	52.46	46.12	57.01	38.23
R _{sf} (Ω)	-	56.02	-	20.33	-	-	-	-

Table S2. The comparisons of the TiS₂-VF/Celgard and TiS₂-SC/Celgard-based Li-S batteries with the recent reports of Li-S batteries with modified separations.

Separator	Host	Sulfur loading (mg cm ⁻²)	Sulfur content (wt%)	Initial capacity (mAh g ⁻¹)	Rate (C)	Cycles	Capacity decay (%)	Ref.
Ketjen Black/PP	Super P	1.5-2	60	1350	0.5	500	0.09	1
GO/PP	CNT	1.0	63	920	0.1	500	0.23	2
Nafion/PP	CNT	0.53	50	800	1	500	0.08	3
Co ₉ S ₈ /Celgard	Super P	2	70	869	1	1000	0.039	4
Super P/Celgard	active carbon	0.7	70	1008	0.5	200	0.185	5
Ni ₃ (HITP) ₂ /PP	Carbon black	3.5	64	1244	0.2	100	0.085	6
Graphene/PP	CNT	1.8	63	1165	0.5	150	0.16	7
TiN/Celgard	Super P	1.3	70	1032	0.2	400	0.091	8
MoS ₂ /Celgard	Carbon black	-	65	808	0.5	600	0.083	9
SnS ₂ /Celgard	Ketjen black	3.1	70	1300	0.2	150	0.2	10
Ti ₃ C ₂ T _x /Celgard	Ti ₃ C ₂	0.7-1	49	899	0.5	50	0.64	11
SnO ₂ @rGO/Celgard	Carbon black	2.87	55	~990	1	200	0.13	12
BaTiO ₃ /Celgard	Ketjen black	3.0	60	1122.1	0.1	50	0.34	13
MOF/Celgard	carbon black	0.6-0.8	70	1126	0.5	500	0.058	14
TiS ₂ -SC/Celgard	Ketjen black	1.8	50	811.2	1	500	0.056	This work
TiS ₂ -VF/Celgard	Ketjen black	1.8	50	887.3	1	500	0.024	This work

References

1. H. Yao, K. Yan, W. Li, G. Zheng, D. Kong, Z. W. Seh, V. K. Narasimhan, Z. Liang and Y. Cui, *Energy Environ. Sci.*, 2014, **7**, 3381-3390.
2. J. Q. Huang, T. Z. Zhuang, Q. Zhang, H. J. Peng, C. M. Chen, F. Wei, *ACS Nano*, 2015, **9**, 3002.
3. J.-Q. Huang, Q. Zhang, H.-J. Peng, X.-Y. Liu, W.-Z. Qian and F. Wei, *Energy Environ. Sci.*, 2014, **7**, 347-353.
4. J. He, Y. Chen and A. Manthiram, *Energy & Environmental Science*, 2018, **11**, 2560-2568.
5. Zhu, J.; Ge, Y.; Kim, D.; Lu, Y.; Chen, C.; Jiang, M.; Zhang, X., *Nano Energy* 2016, **20**, 176–184.
6. Y. Zang, F. Pei, J. Huang, Z. Fu, G. Xu and X. Fang, *Advanced Energy Materials*, 2018, **8**, 1802052.
7. P.-Y. Zhai, H.-J. Peng, X.-B. Cheng, L. Zhu, J.-Q. Huang, W. Zhu and Q. Zhang, *Energy Storage Materials*, 2017, **7**, 56-63.
8. B. Qi, X. Zhao, S. Wang, K. Chen, Y. Wei, G. Chen, Y. Gao, D. Zhang, Z. Sun and F. Li, *Journal of Materials Chemistry A*, 2018, **6**, 14359-14366.
9. Z. A. Ghazi, X. He, A. M. Khattak, N. A. Khan, B. Liang, A. Iqbal, J. Wang, H. Sin, L. Li and Z. Tang, *Advanced materials*, 2017, **29**.
10. B. Moorthy, S. Kwon, J. H. Kim, P. Ragupathy, H. M. Lee and D. K. Kim, *Nanoscale Horiz*, 2019, **4**, 214-222.
11. Y. Dong, S. Zheng, J. Qin, X. Zhao, H. Shi, X. Wang, J. Chen and Z. S. Wu, *ACS nano*, 2018, **12**, 2381-2388.
12. N. Hu, X. Lv, Y. Dai, L. Fan, D. Xiong and X. Li, *ACS applied materials & interfaces*, 2018, **10**, 18665-18674.
13. T. Yim, S. H. Han, N. H. Park, M.-S. Park, J. H. Lee, J. Shin, J. W. Choi, Y. Jung, Y. N. Jo, J.-S. Yu and K. J. Kim, *Advanced Functional Materials*, 2016, **26**, 7817-7823.
14. S. Bai, X. Liu, K. Zhu, S. Wu and H. Zhou, *Nature Energy*, 2016, **1**.