

Supporting Information

Metallic 1T phase MoS₂ nanosheets decorated hollow cobalt sulfide polyhedrons for high-performance lithium storage

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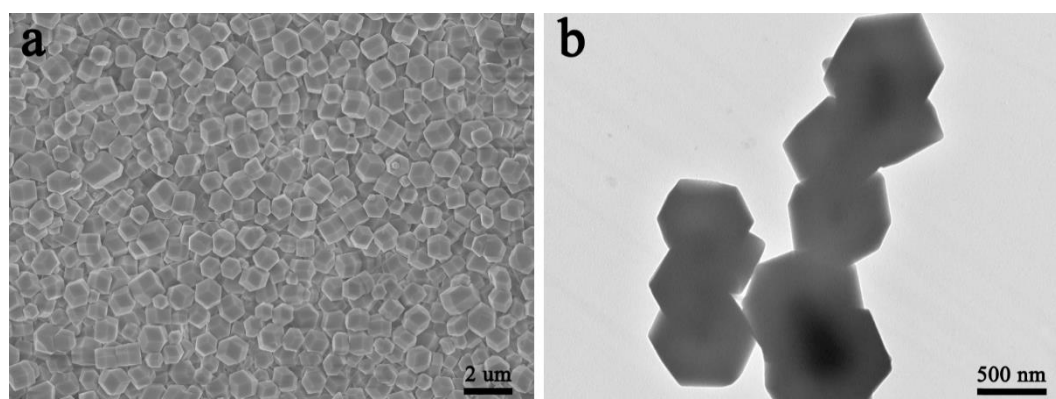


Figure S1. (a) FESEM and (b) TEM graphs of ZIF-67.

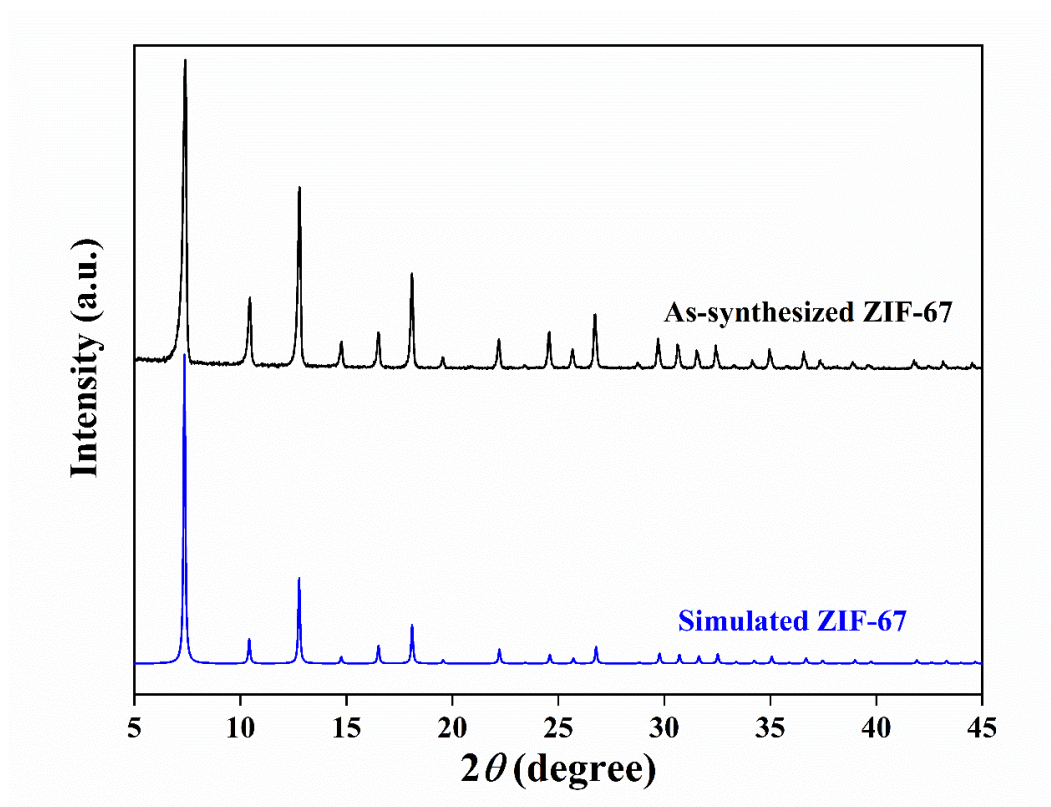


Figure S2. XRD patterns of the as-synthesized ZIF-67 and simulated ZIF-67.

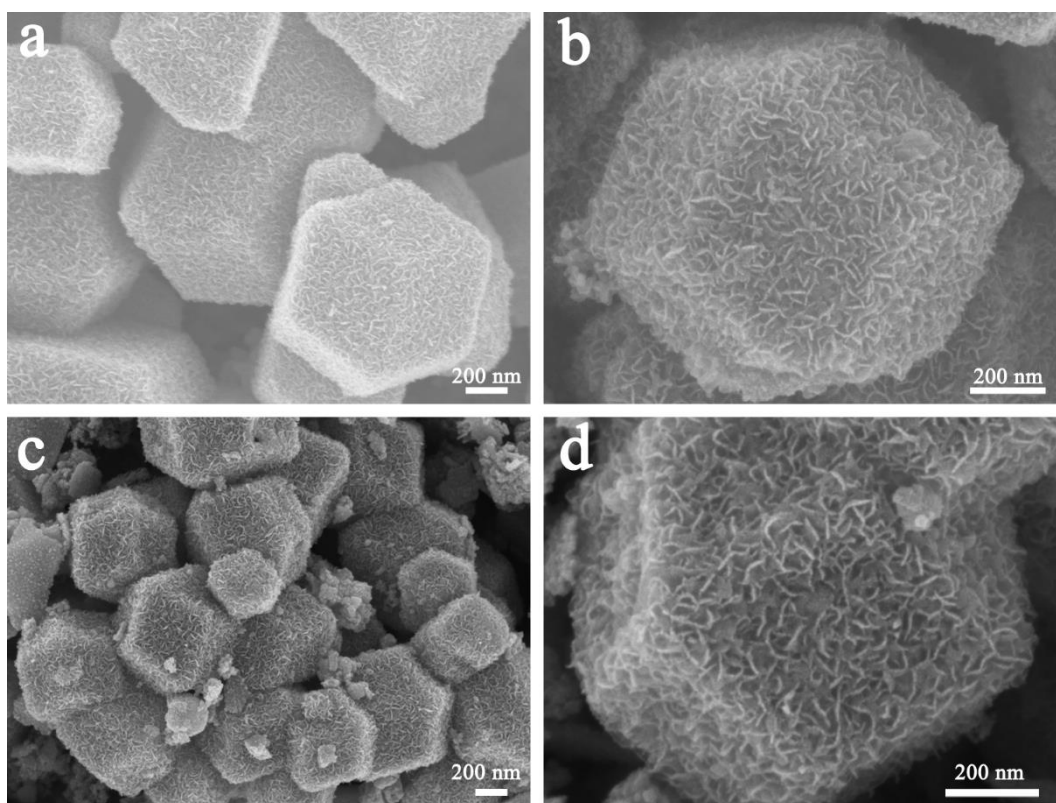


Figure S3. SEM images of (a, b) CoS@1T-MoS₂ and (c, d) Co₉S₈@2H-MoS₂.

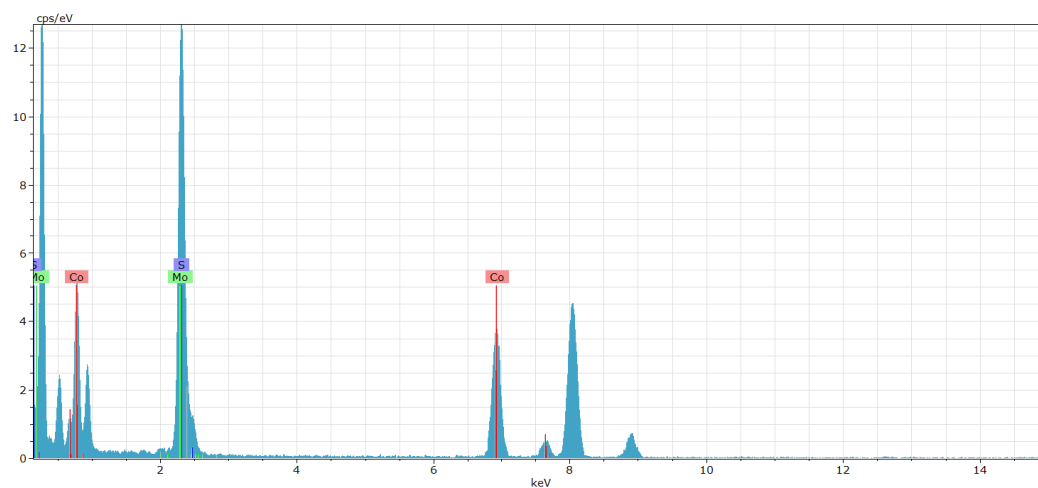


Figure S4. EDX spectrum of CoS@1T-MoS₂.

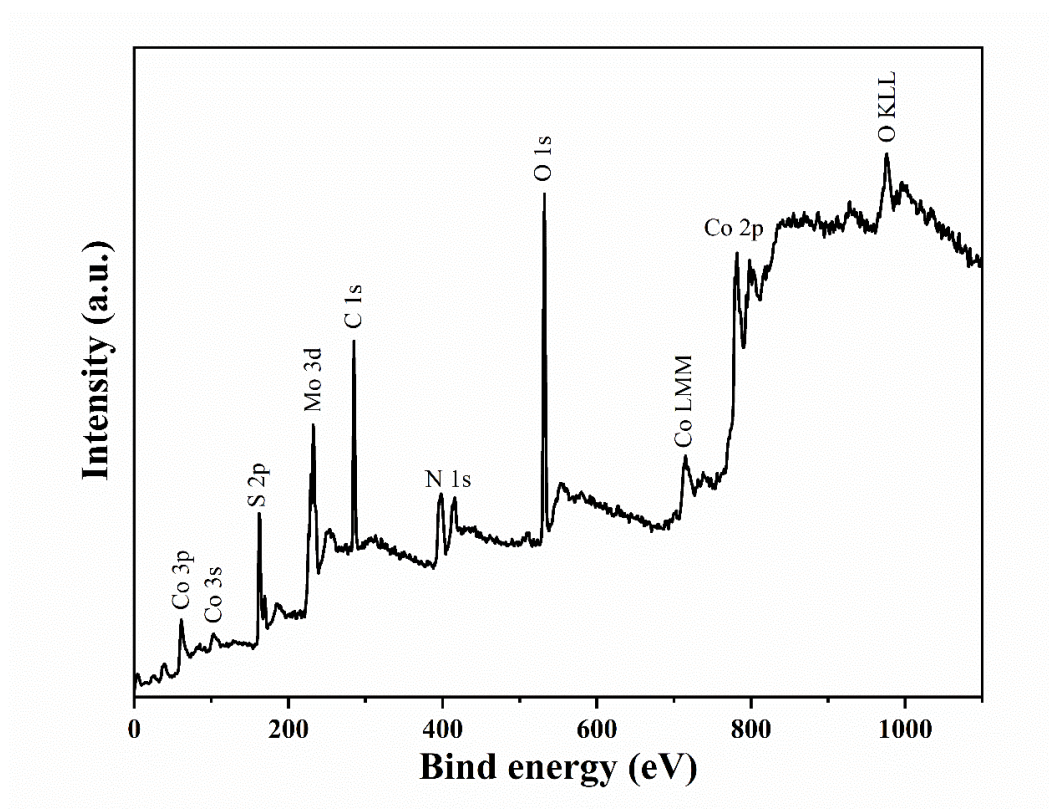


Figure S5. XPS wide scan spectral plot of CoS@1T-MoS₂.

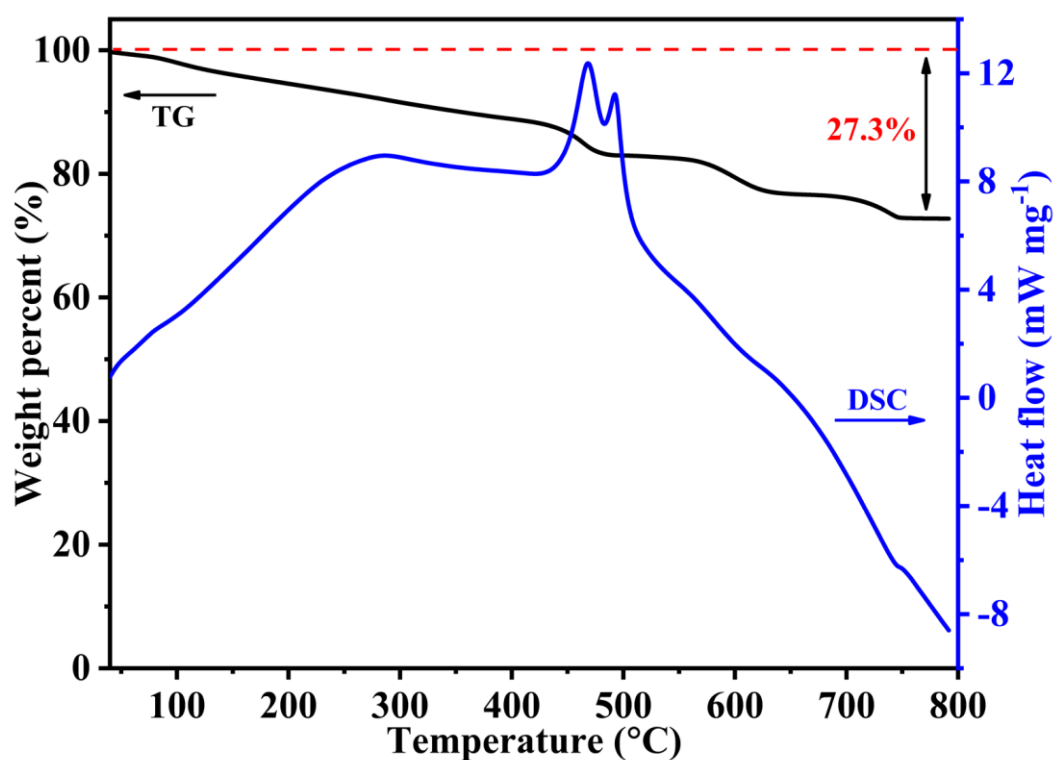


Figure S6. TGA-DSC curve of CoS@1T-MoS₂ in air.

Based on the TGA-DSC and ICP results (**Table. S1, ESI†**), the mass contents of MoS₂, CoS and amorphous carbon in the composite can be roughly calculated to be 59.0%, 34.7%, and 6.3%, respectively.

Table S1. ICP result of the CoS@1T-MoS₂ composite.

Element	Mass concentration	Mass ratio
Co	47.66μg/mL	1
Mo	74.38μg/mL	1.56

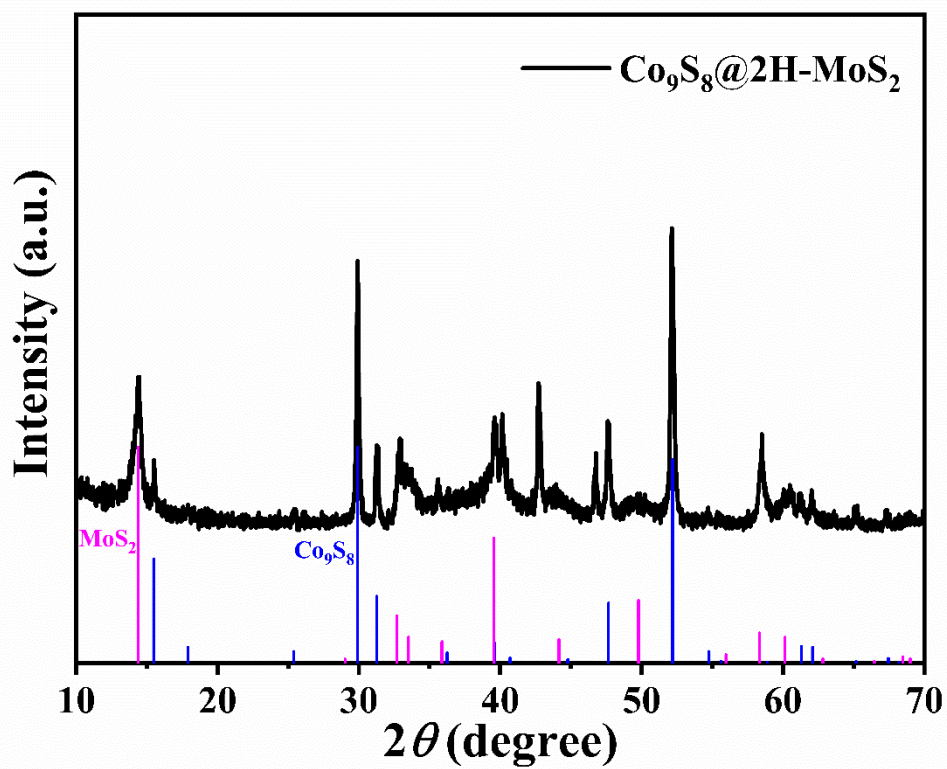


Figure S7. XRD patterns of $\text{Co}_9\text{S}_8@2\text{H-MoS}_2$.

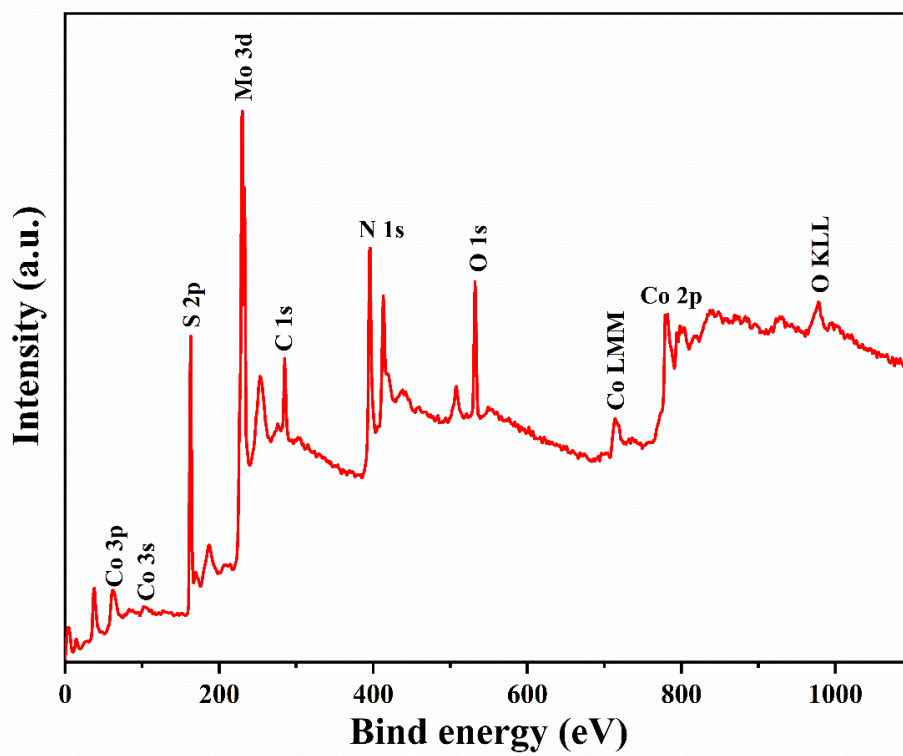


Figure S8. XPS wide scan spectral plot of $\text{Co}_9\text{S}_8@2\text{H-MoS}_2$.

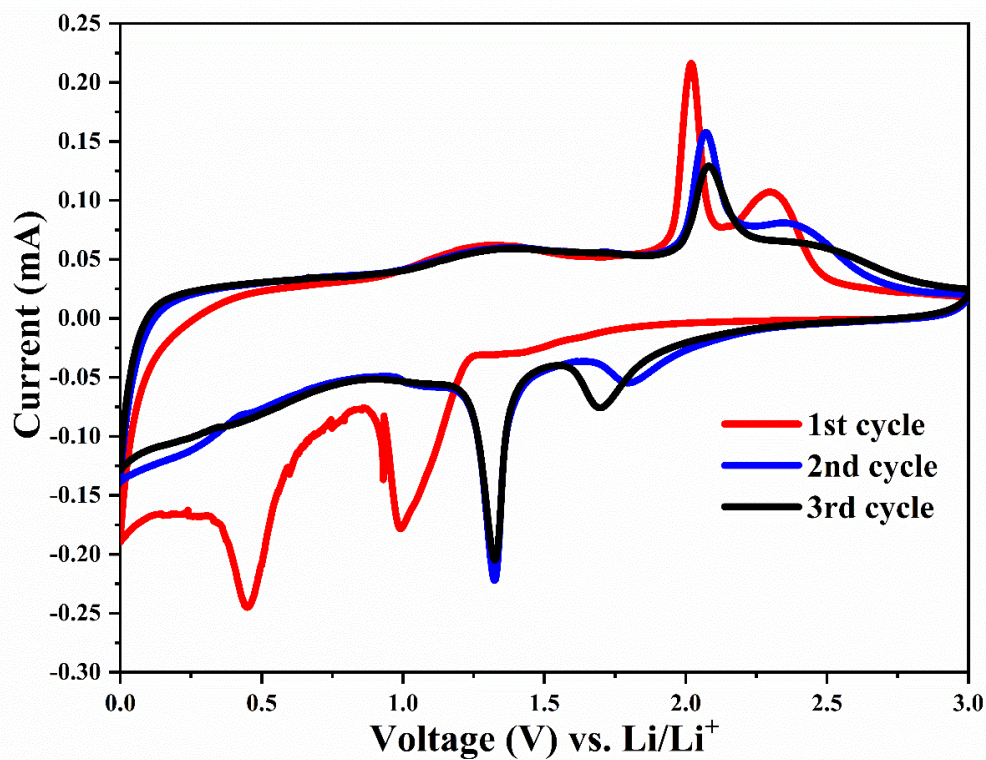


Figure S9. CV curve of the first three cycles of $\text{Co}_9\text{S}_8@2\text{H-MoS}_2$ in a voltage range of 0.0–3.0 V at a scan rate of 0.1 mV s^{-1} .

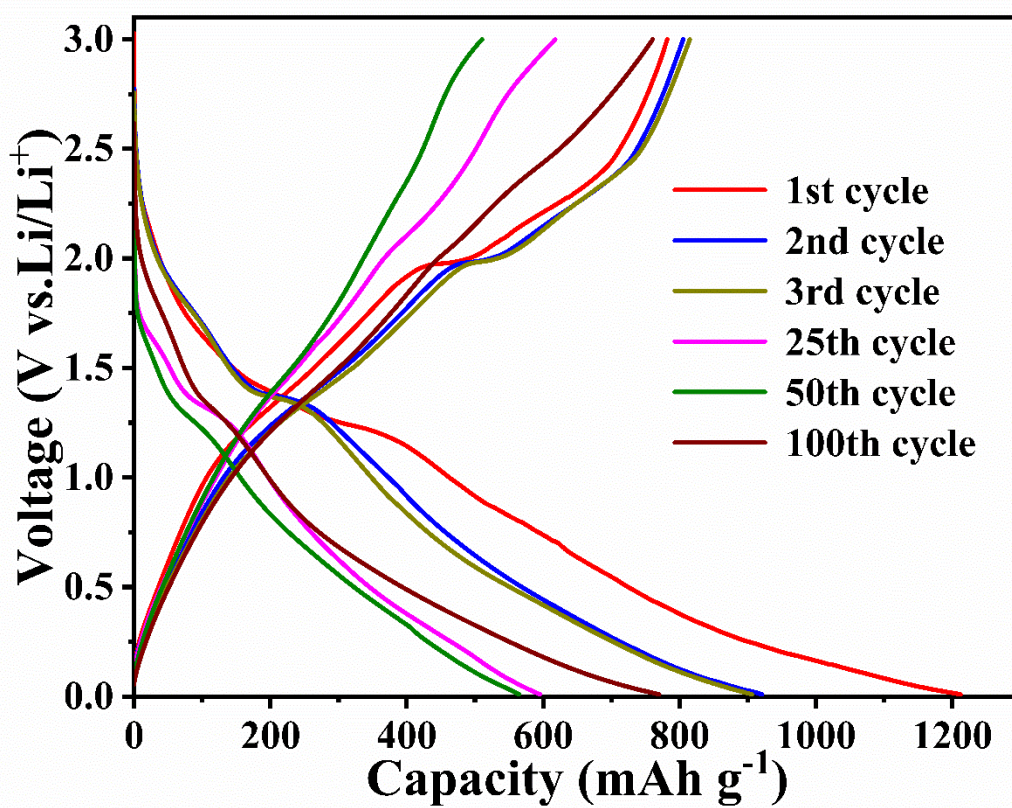


Figure S10. Charge/discharge voltage profiles of the $\text{Co}_9\text{S}_8@2\text{H-MoS}_2$ electrode for the 1st, 2nd, 3rd, 25th, 50th, and 100th cycles at a current density of 0.1 A g^{-1} .

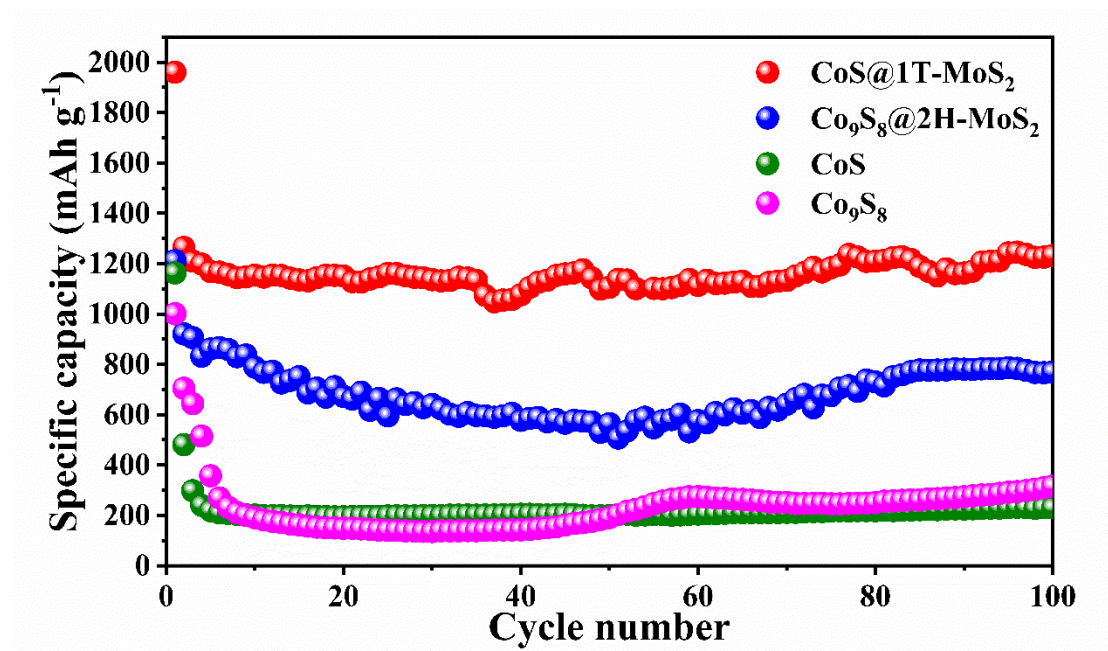


Figure S11. Cycling performance of the CoS@1T-MoS_2 , $\text{Co}_9\text{S}_8@2\text{H-MoS}_2$, CoS and Co_9S_8 electrodes at a current density of 0.1 A g^{-1} .

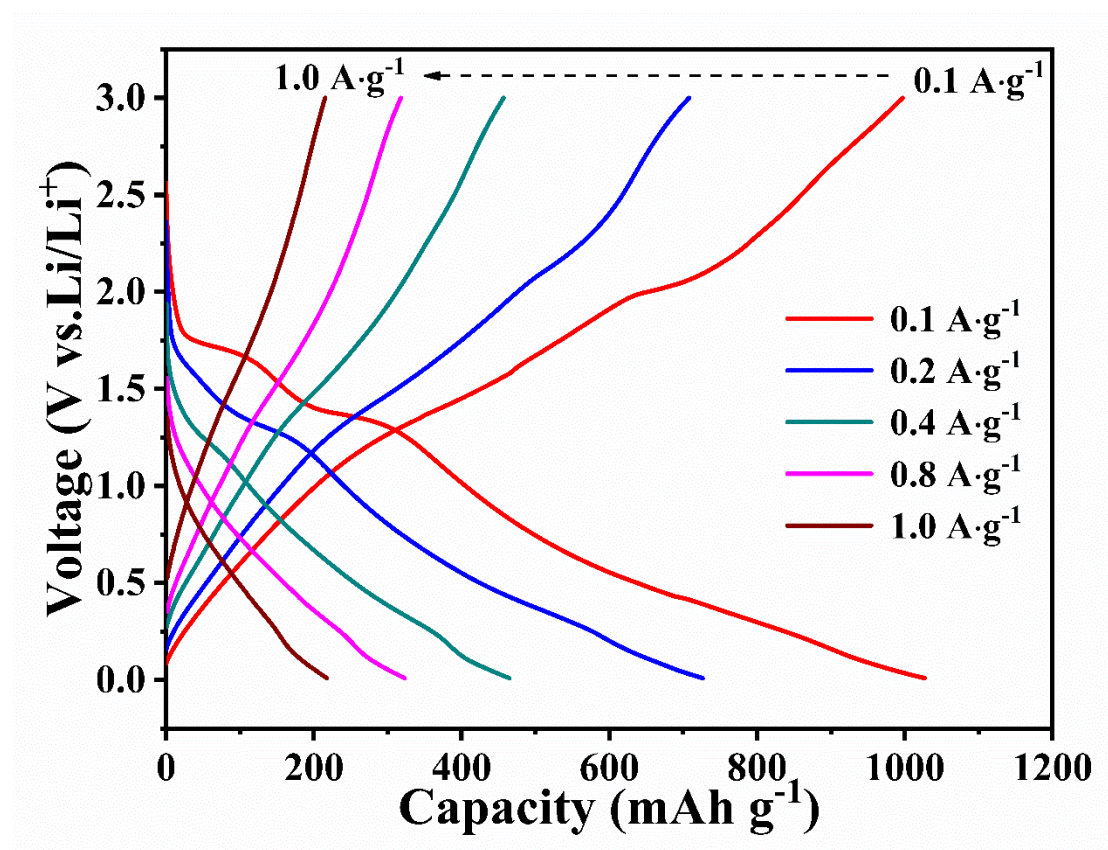


Figure S12. Charge/discharge profiles of the $\text{Co}_9\text{S}_8@2\text{H-MoS}_2$ electrode at different

rate current densities.

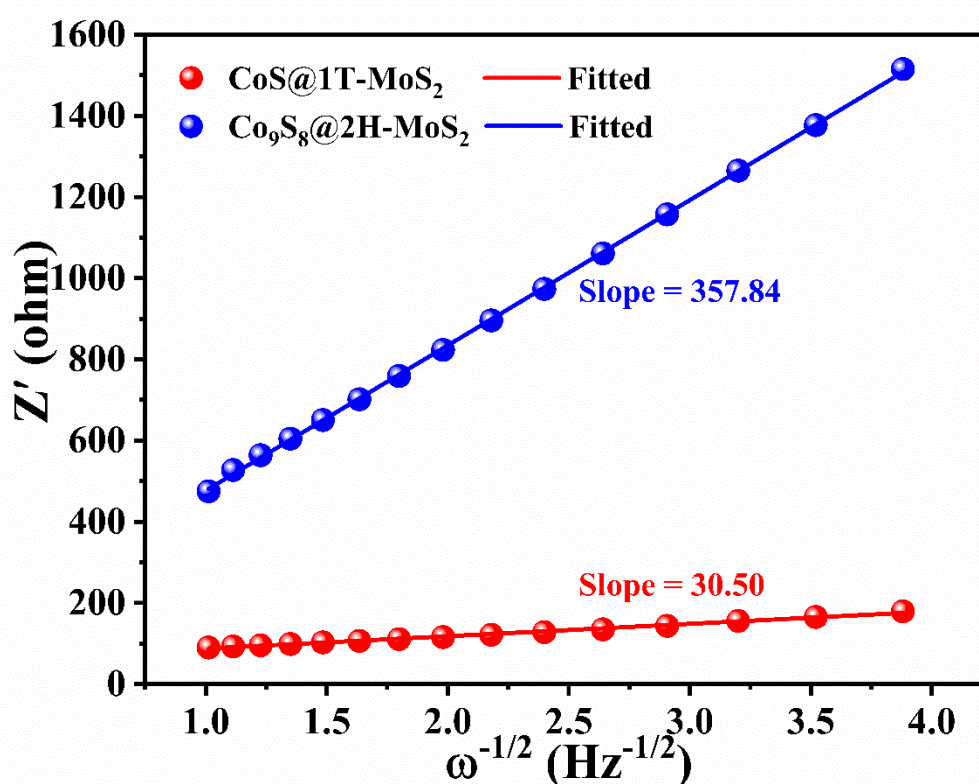


Figure S13. Fitted straight lines of Z' vs. $\omega^{-1/2}$ at low frequency of CoS@1T-MoS₂ and Co₉S₈@2H-MoS₂.

The lithium ion diffusion coefficient can be calculated using the following equation:¹

$$D = \frac{R^2 T^2}{2 A^2 n^4 F^4 C^2 \sigma^2}$$

where D is the diffusion coefficient, R is the gas constant, T is the absolute temperature, A is the surface area of the electrode, n is the number of the electrons per molecule attending the electronic transfer reaction, F is the Faraday constant, C is the concentration of lithium ion in the electrode, σ is the Warburg factor which can be calculated from the slope of the line $Z' \sim \omega^{-1/2}$ (shown in **Fig. S13, ESI†**), respectively.

The calculated lithium diffusion coefficient of the CoS@1T-MoS₂ electrode is $2.35 \times 10^{-11} \text{ cm}^2 \text{ s}^{-1}$, almost 138 times higher than that of the Co₉S₈@2H-MoS₂ electrode ($1.70 \times 10^{-13} \text{ cm}^2 \text{ s}^{-1}$).

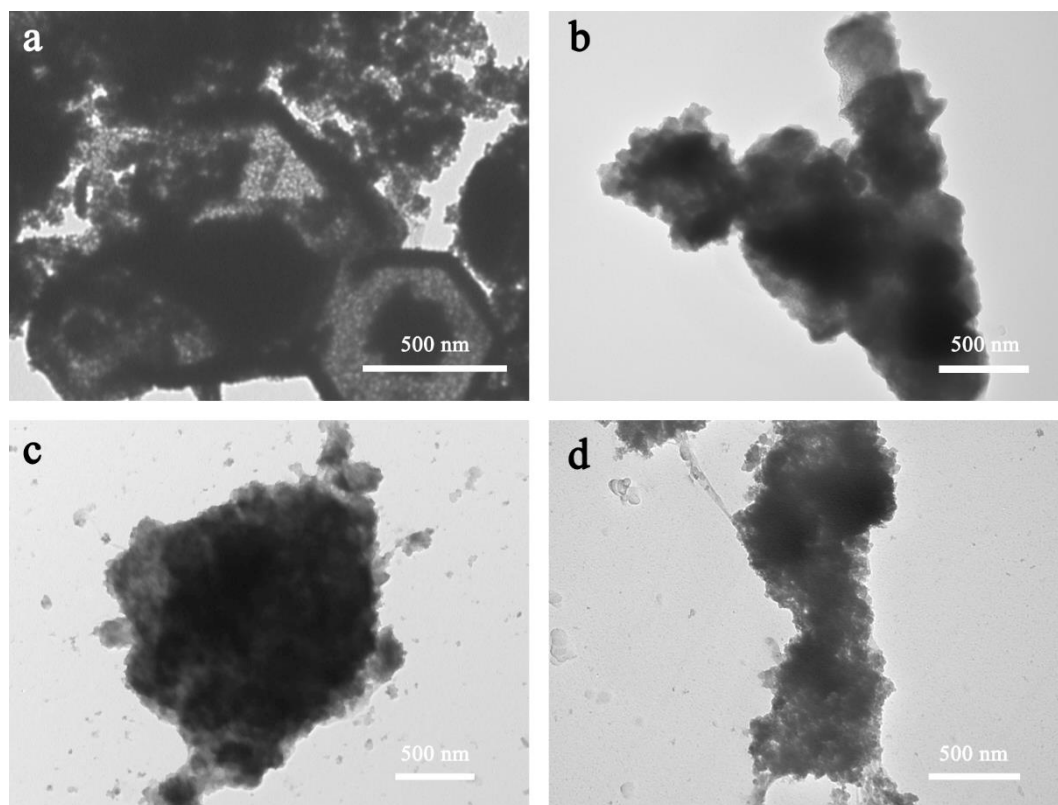


Figure S14. TEM image of the CoS@1T-MoS₂ composite after 100 cycles at a current density of 0.1 A g⁻¹ (a) and 220 cycles at a current density of 1 A g⁻¹ (b-d).

Table S2. The comparison of Li-storage performance between CoS@1T-MoS₂ and other CoS_x-based anodes.

Samples	Current density (mA g ⁻¹)	Charge capacity (mA h g ⁻¹)	Cycle number	Ref.
Co ₉ S ₈ /N-C	544	784	400	2
rGO/CoS _x	100	613	100	3
NiS ₂ @CoS ₂	1000	670	100	4
CoS ₂ /rGO	50	644	30	5
CoS ₂	100	720	10	6
CoS	100	589	10	6
M-CoS@C	1000	790	500	7
CoS/graphene	58.9	898	80	8
CoS@PCP/CNTs	200	1668	100	9
Co ₉ S ₈ /MoS ₂	1000	732	200	10
Co ₃ S ₄ /Graphene	140.56	720	100	11
NC/CoS ₂ -650	100	560	50	12
CoS _x hollow spheres	500	1012	100	13
Co ₉ S ₈ hollow spheres	100	254.9	100	14
Flower-like Co _{1-x} S	100	485	150	15
Yolk shell Co ₉ S ₈	1000	634	100	16

Rose-like Co ₉ S ₈	50	123	30	17
Graphene/Co ₉ S ₈	545	573	500	18
MWCNT@a-C@Co ₉ S ₈	1000	662	120	19
CoS@1T-MoS₂	100	1269	100	This
	1000	936	220	work

Table S3. The comparison of Li-storage performance between CoS@1T-MoS₂ and other MoS₂-based anodes.

Samples	Current density (mA g ⁻¹)	Charge capacity (mA h g ⁻¹)	Cycle number	Ref.
Hollow MoS ₂ nanotubes	100	727	100	20
MoS ₂ /C	100	888.1	50	21
Hollow MoS ₂ nanoparticles	100	902	80	22
MoS ₂ -SWNT	100	992	100	23
Single-layer MoS ₂ -graphene nanosheet	100	808	100	24
Quasi-hollow C@MoS ₂	100	652	100	25
FL-MoS ₂ @PCNNs	2000	676	520	26
MoS ₂ /mesoporous carbon	400	1023	500	27
Co ₉ S ₈ /MoS ₂	1000	732	200	10
MoS ₂ -C microspheres	1000	800	170	28
C@MoS ₂ nanoboxes	100	900	50	29
MoS ₂ /Polyaniline nanowires	100	952.6	50	30
MoS ₂ /N-doped graphene nanosheets	100	1021.2	50	31
CNT/MoS ₂ tubular nanohybrids	5000	800	1000	32
MoS ₂ @Carbon microspheres	1000	650	300	33
MoS ₂ entrapped carbon sheath	1000	823	200	34
MoS ₂ /Nanotube Composite	2000	950	500	35
MoS ₂ /rGO nanoflowers	100	1150	60	36
Yolk/shell MoS ₂ @C	1000	993	200	37
HC-MoS ₂ @GF	200	820	50	38
Single-layered MoS ₂ /carbon nanowire	1000	1007	100	39
1T-MoS ₂ /CFC	1000	853	140	40
CoS@1T-MoS₂	100	1269	100	This
	1000	936	220	work

References

1. X. Y. Wang, H. Hao, J. L. Liu, T. Huang and A. S. Yu, *Electrochim Acta*, 2011, **56**, 4065-4069.
2. P. Y. Zeng, J. W. Li, M. Ye, K. F. Zhuo and Z. Fang, *Chem-Eur J*, 2017, **23**, 9517-9524.
3. D. M. Yin, G. Huang, F. F. Zhang, Y. L. Qin, Z. L. Na, Y. M. Wu and L. M. Wang, *Chem-Eur J*, 2016, **22**, 1467-1474.
4. Y. Lin, Z. Qiu, D. Li, S. Ullah, Y. Hai, H. Xin, W. Liao, B. Yang, H. Fan, J. Xu and C. Zhu, *Energy Storage Materials*, 2018, **11**, 67-74.
5. Q. M. Su, J. Xie, J. Zhang, Y. J. Zhong, G. H. Du and B. S. Xu, *Acs Appl Mater Inter*, 2014, **6**, 3016-3022.
6. Y. Wang, J. J. Wu, Y. F. Tang, X. J. Lii, C. Y. Yang, M. S. Qin, F. Q. Huang, X. Li and X. Zhang, *Acs Appl Mater Inter*, 2012, **4**, 4246-4250.
7. Q. D. Li, L. Li, K. A. Owusu, W. Luo, Q. Y. An, Q. L. Wei, Q. J. Zhang and L. Q. Mai, *Nano Energy*, 2017, **41**, 109-116.
8. S. F. Kong, Z. T. Jin, H. Liu and Y. Wang, *J Phys Chem C*, 2014, **118**, 25355-25364.
9. R. B. Wu, D. P. Wang, X. H. Rui, B. Liu, K. Zhou, A. W. K. Law, Q. Y. Yan, J. Wei and Z. Chen, *Advanced Materials*, 2015, **27**, 3038-3044.
10. H. Geng, J. Yang, Z. Dai, Y. Zhang, Y. Zheng, H. Yu, H. Wang, Z. Luo, Y. Guo, Y. Zhang, H. Fan, X. Wu, J. Zheng, Y. Yang, Q. Yan and H. Gu, *Small*, 2017, **13**.
11. N. Mahmood, C. Z. Zhang, J. Jiang, F. Liu and Y. L. Hou, *Chem-Eur J*, 2013, **19**, 5183-5190.
12. Q. F. Wang, R. Q. Zou, W. Xia, J. Ma, B. Qiu, A. Mahmood, R. Zhao, Y. Y. C. Yang, D. G. Xia and Q. Xu, *Small*, 2015, **11**, 2511-2517.
13. Y. Xiao, J. Y. Hwang, I. Belharouak and Y. K. Sun, *Nano Energy*, 2017, **32**, 320-328.
14. R. C. Jin, J. H. Zhou, Y. S. Guan, H. Liu and G. Chen, *Journal of Materials Chemistry A*, 2014, **2**, 13241-13244.
15. S. M. Liu, J. X. Wang, J. W. Wang, F. F. Zhang, F. Liang and L. M. Wang, *Crystengcomm*, 2014, **16**, 814-819.
16. Y. N. Ko, S. H. Choi, S. B. Park and Y. C. Kang, *Chem-Asian J*, 2014, **9**, 572-576.
17. R. C. Jin, J. S. Liu, Y. B. Xu, G. H. Li and G. Chen, *Journal of Materials Chemistry A*, 2013, **1**, 7995-7999.
18. H. H. Wang, S. T. Lu, Y. Chen, L. Han, J. Zhou, X. H. Wu and W. Qin, *Journal of Materials Chemistry A*, 2015, **3**, 23677-23683.
19. Y. L. Zhou, D. Yan, H. Y. Xu, S. Liu, J. Yang and Y. T. Qian, *Nanoscale*, 2015, **7**, 3520-3525.
20. G. D. Li, X. Y. Zeng, T. D. Zhang, W. Y. Ma, W. P. Li and M. Wang, *Crystengcomm*, 2014, **16**, 10754-10759.
21. L. R. Hu, Y. M. Ren, H. X. Yang and Q. Xu, *Acs Appl Mater Inter*, 2014, **6**, 14644-14652.
22. M. Wang, G. D. Li, H. Y. Xu, Y. T. Qian and J. Yang, *Acs Appl Mater Inter*, 2013, **5**, 1003-1008.
23. J. Z. Wang, L. Lu, M. Lotya, J. N. Coleman, S. L. Chou, H. K. Liu, A. I. Minett and J. Chen, *Advanced Energy Materials*, 2013, **3**, 798-805.
24. Z. Wang, T. Chen, W. X. Chen, K. Chang, L. Ma, G. C. Huang, D. Y. Chen and J. Y. Lee, *Journal of Materials Chemistry A*, 2013, **1**, 2202-2210.
25. Z. M. Wan, J. Shao, J. J. Yun, H. Y. Zheng, T. Gao, M. Shen, Q. T. Qu and H. H. Zheng, *Small*, 2014, **10**, 4975-4981.
26. J. W. Zhou, J. Qin, X. Zhang, C. S. Shi, E. Z. Liu, J. J. Li, N. Q. Zhao and C. N. He, *Acs Nano*, 2015,

- 9, 3837-3848.
27. H. Jiang, D. Y. Ren, H. F. Wang, Y. J. Hu, S. J. Guo, H. Y. Yuan, P. J. Hu, L. Zhang and C. Z. Li, *Advanced Materials*, 2015, **27**, 3687-3695.
 28. G. Chen, S. P. Wang, R. Yi, L. F. Tan, H. B. Li, M. Zhou, L. T. Yan, Y. B. Jiang, S. Tan, D. H. Wang, S. G. Deng, X. W. Meng and H. M. Luo, *Journal of Materials Chemistry A*, 2016, **4**, 9653-9660.
 29. L. Zhang, H. B. Wu, Y. Yan, X. Wang and X. W. Lou, *Energ Environ Sci*, 2014, **7**, 3302-3306.
 30. L. C. Yang, S. N. Wang, J. J. Mao, J. W. Deng, Q. S. Gao, Y. Tang and O. G. Schmidt, *Advanced Materials*, 2013, **25**, 1180-1184.
 31. K. Chang, D. S. Geng, X. F. Li, J. L. Yang, Y. J. Tang, M. Cai, R. Y. Li and X. L. Sun, *Advanced Energy Materials*, 2013, **3**, 839-844.
 32. Y. M. Chen, X. Y. Yu, Z. Li, U. Paik and X. W. Lou, *Sci Adv*, 2016, **2**.
 33. Z. C. Bai, Y. H. Zhang, Y. W. Zhang, C. L. Guo and B. Tang, *Chem-Eur J*, 2015, **21**, 18187-18191.
 34. Z. Sun, Y. C. Yao, J. Wang, X. F. Song, P. Zhang, L. P. Zhao and L. Gao, *Journal of Materials Chemistry A*, 2016, **4**, 10425-10434.
 35. Y. P. Liu, X. Y. He, D. Hanlon, A. Harvey, U. Khan, Y. G. Li and J. N. Coleman, *Acs Nano*, 2016, **10**, 5980-5990.
 36. H. L. Li, K. Yu, H. Fu, B. J. Guo, X. Lei and Z. Q. Zhu, *J Phys Chem C*, 2015, **119**, 7959-7968.
 37. X. Zhang, R. F. Zhao, Q. H. Wu, W. L. Li, C. Shen, L. B. Ni, H. Yan, G. W. Diao and M. Chen, *Acs Nano*, 2017, **11**, 8429-8436.
 38. J. Wang, J. L. Liu, D. L. Chao, J. X. Yan, J. Y. Lin and Z. X. Shen, *Advanced Materials*, 2014, **26**, 7162-7169.
 39. C. B. Zhu, X. K. Mu, P. A. van Aken, Y. Yu and J. Maier, *Angew Chem Int Edit*, 2014, **53**, 2152-2156.
 40. M. H. Wu, J. Zhan, K. Wu, Z. Li, L. Wang, B. J. Geng, L. J. Wang and D. Y. Pan, *Journal of Materials Chemistry A*, 2017, **5**, 14061-14069.