Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.


# Supplementary Information

## In-situ growth of tungsten carbide nanoparticles on nanocarbon as electrocatalyst promotes redox reaction kinetics of high mass loading sulfur cathode for high volumetric performance

Jing Zhang [a,†], Shaorong Duan [b,†] Caiyin You [a*], Jian Wang [c], Haitao Liu [d], Shaohua Guo [a], Weihua Zhang [a], Rong Yang [e]

[a] *School of Materials Science and Engineering, Xi'an University of Technology, Xi'an 710048, P. R. China*

[b] *State Key Laboratory of Low Dimensional Quantum Physics and Department of Physics, Tsinghua University, Beijing, 100084, China*

[c] *i-Lab, Suzhou Institute of Nano-Tech and Nano-Bionics, Chinese Academy of Sciences, Suzhou, Jiangsu, 215123, P. R. China*

[d] *Laboratory of Computational Physics, Institute of Applied Physics and Computational Mathematics, Beijing, 100088, China*

[e] *School of Sciences, Xi'an University of Technology, Xi'an 710048, P. R. China*

* Corresponding author: caiyinyou@xaut.edu.cn

† These authors contributed equally to this work.

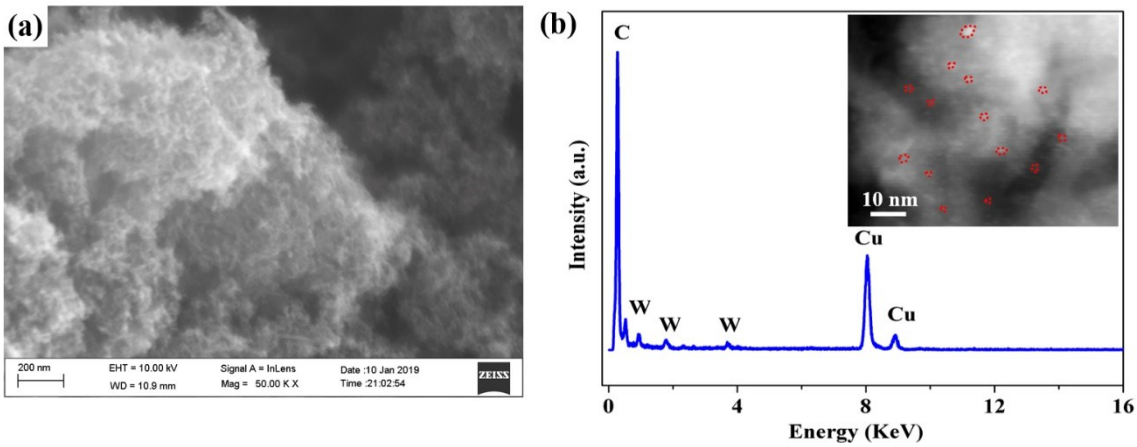


**Fig. S1** (a) SEM image of HCPC; (b) Component analysis from the bright spots in the ADF-TEM image of WCNP@HCPC (the inset).

Fig. S1 (b) shows the energy-dispersive X-ray spectrum (EDX) of WC NPs (the bright spots highlighted by red dashed line) from the scanning TEM (STEM) image. The characteristic peaks of W and C are perfectly assigned to the WC NPs, while the peaks of Cu are attributed to the sample grid.

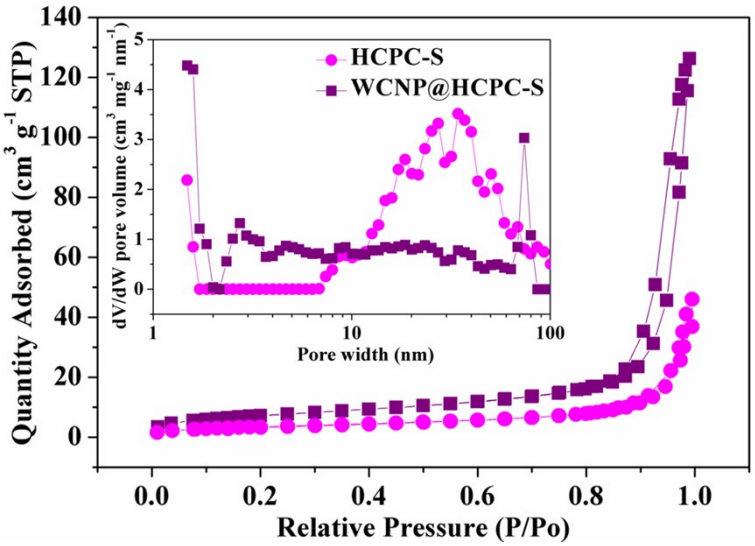


**Fig. S2** $N_2$ adsorption/desorption isotherms and the inset of the pore size distribution of WCNP@HCPC-S and HCPC-S composites.

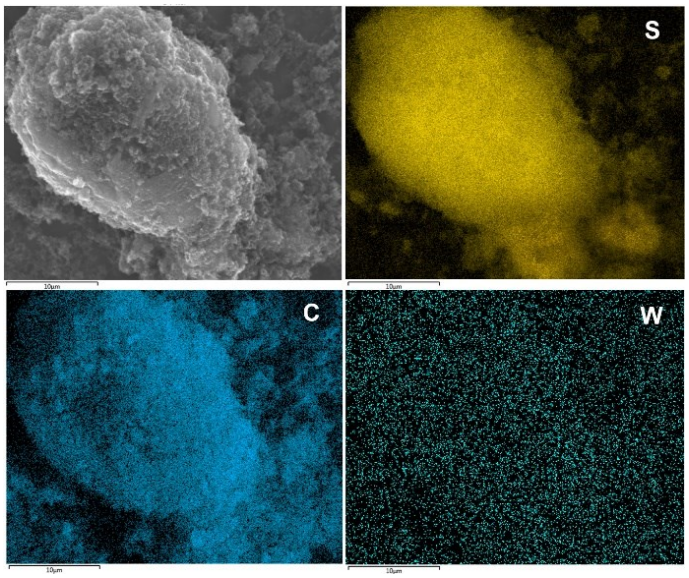


**Fig. S3** Elemental mapping of WCNP@HCPC-S composite, including: elemental sulfur, carbon and tungsten.

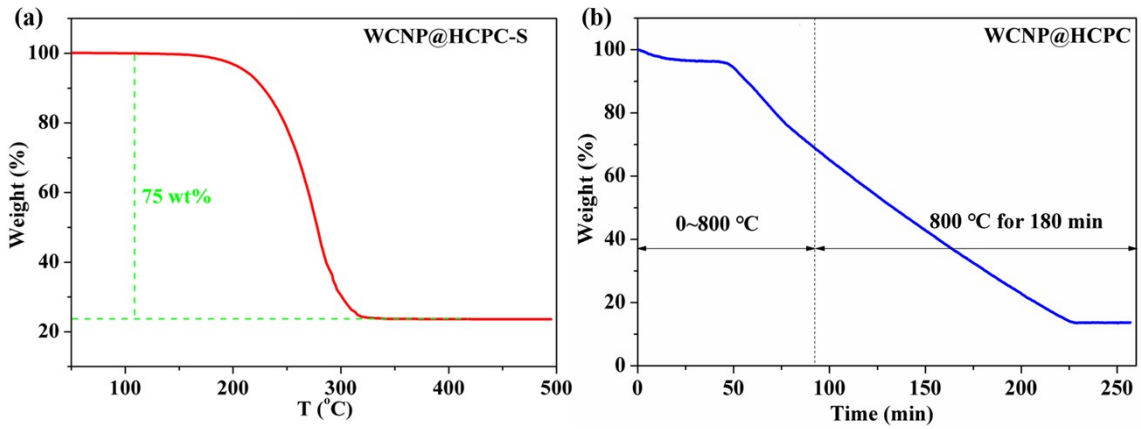


**Fig. S4** (a) TGA curve of WCNP@HCPC-S under $N_2$ flow atmosphere; (b) TGA curve of WCNP@HCPC under $O_2$ flow atmosphere.

The TGA curve of WCNP@HCPC (Fig. S2b) under $O_2$ flow atmosphere reveals the mass residual of 13 wt % after heating. According to the reaction equation (1), the weight of the WC increases to nearly 1.2 times when it is transformed to $WO_3$ under the high temperature heating. Therefore, it could be deduced that the remained mass in Fig. S2b is evaluated to be about 10.5 wt% (12.6% / 1.2) WC. This experimental result matches well with the nominal designed ratio.

$$WC + 2O_2 \xrightarrow{\Delta} WO_3 + CO \quad (1)$$

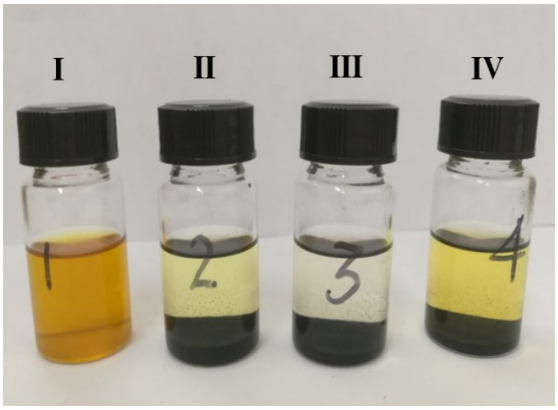


**Fig.S5** Photo image of polysulfide solution after soaking in the adsorbents for 12 h: Ⅰ Control; Ⅱ WCB@HCPC; Ⅲ WCNP@HCPC; Ⅳ HCPC.

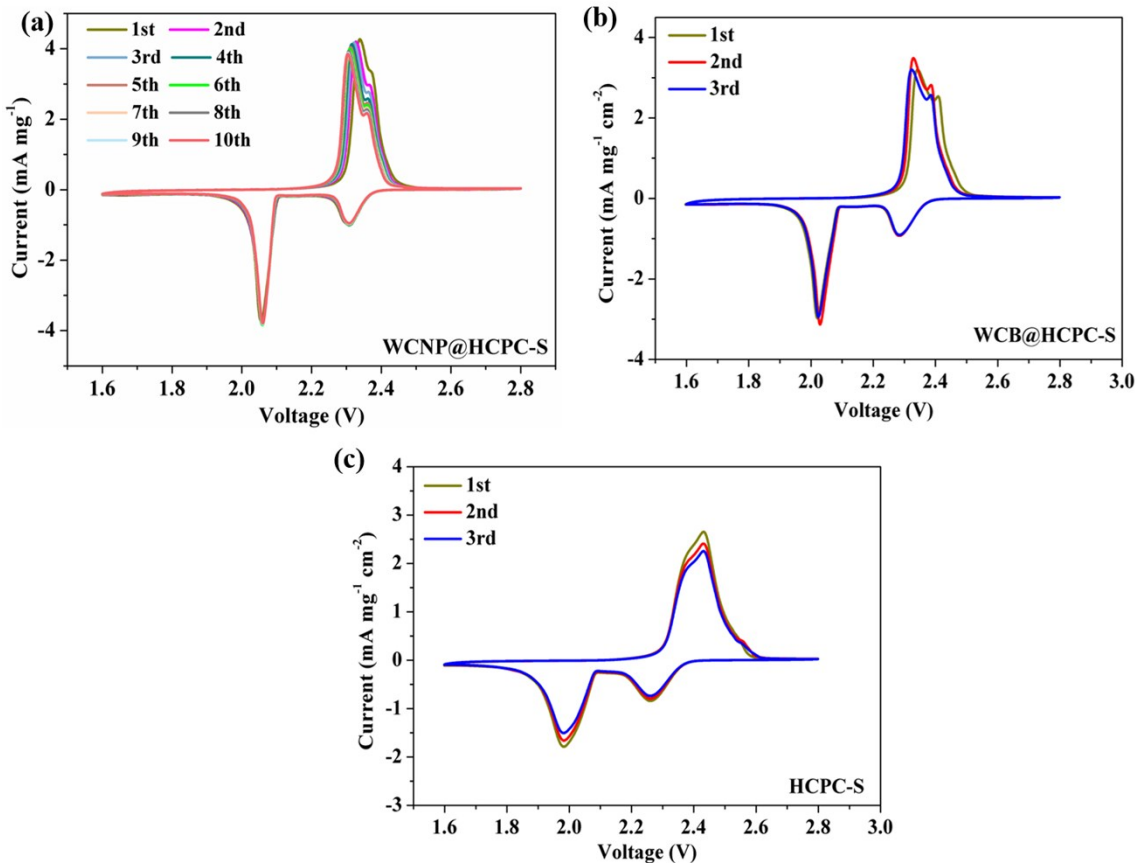


**Fig. S6** Cyclic voltammetry (CV) curves of (a) WCNP@HCPC-S; (b) WCB@HCPC-S and (c) HCPC-S cathodes within the scan range from 1.6 to 2.8V (vs. Li/Li+) at the scan rate of 0.1mV $s^{-1}$.

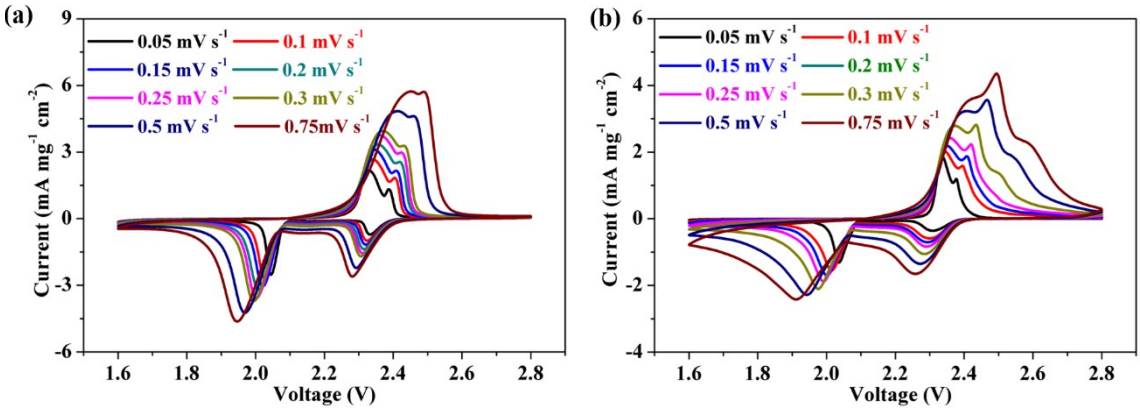


**Fig. S7** CV curves of (a) WCB@HCPC-S and (b) HCPC-S cathodes depending on different scan rates.

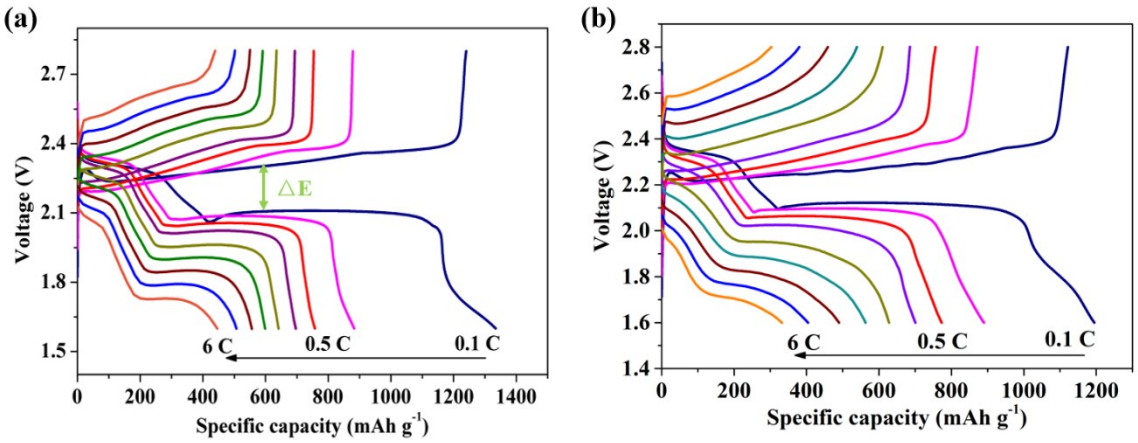


**Fig. S8** Voltage-capacity profiles of (a) WCB@HCPC-S and (b) HCPC-S cathodes at rates varying from 0.1 to 6 C

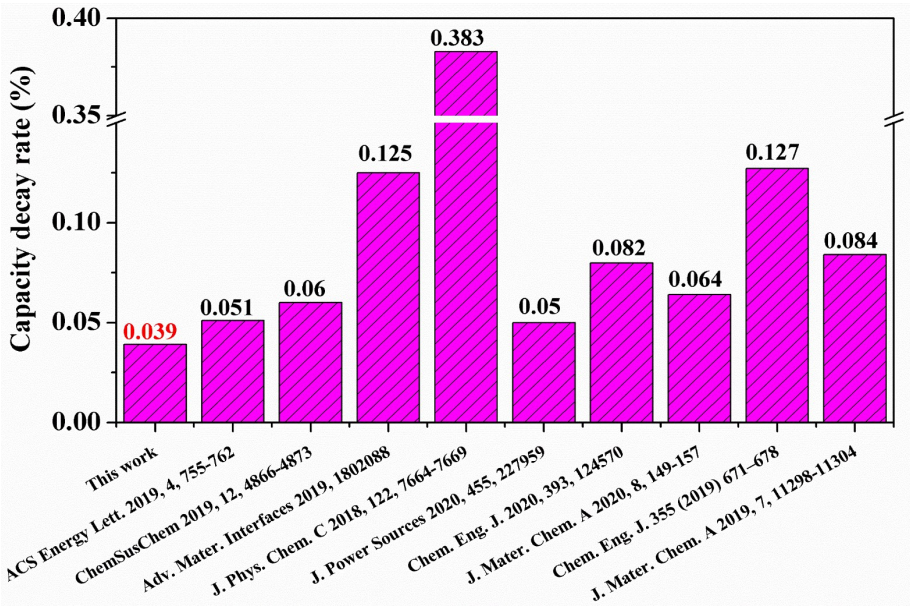


**Fig. S9** Comparison of the capacity decay of this work at high rate with the recent articles

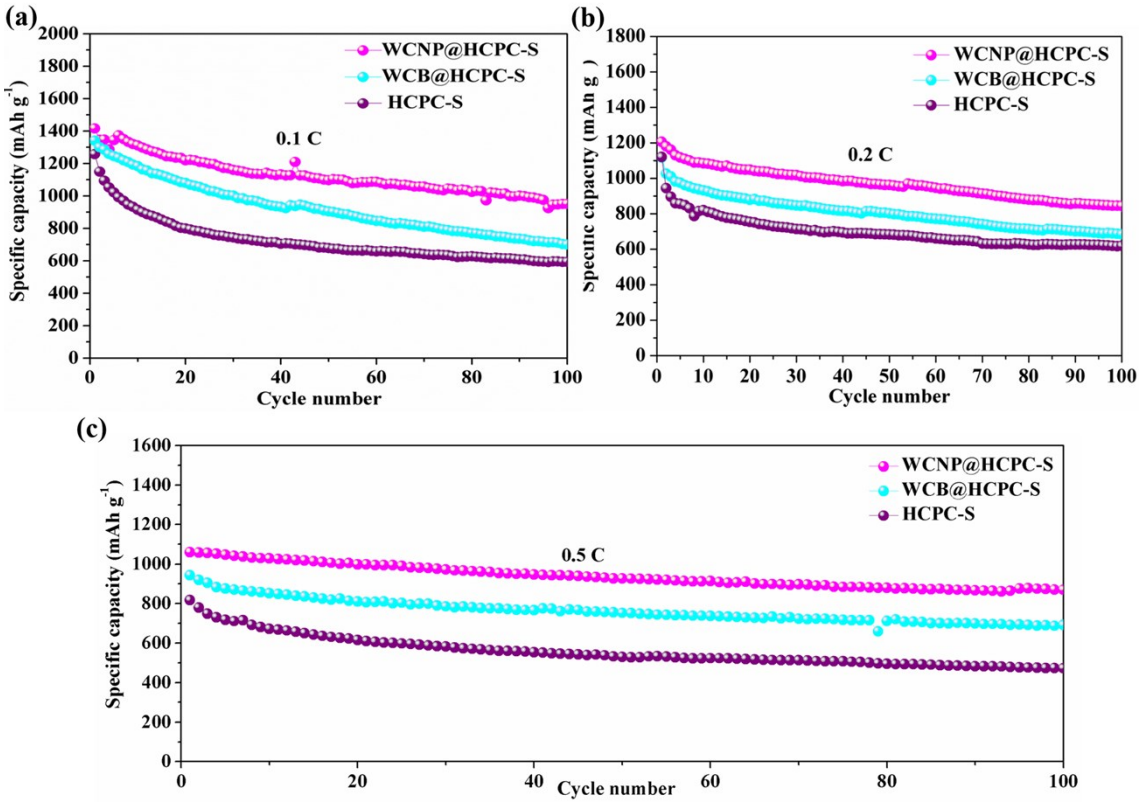


**Fig. S10** Cycle performance of the cathodes at (a) 0.1 C, (b) 0.2 C and (c) 0.5 C.

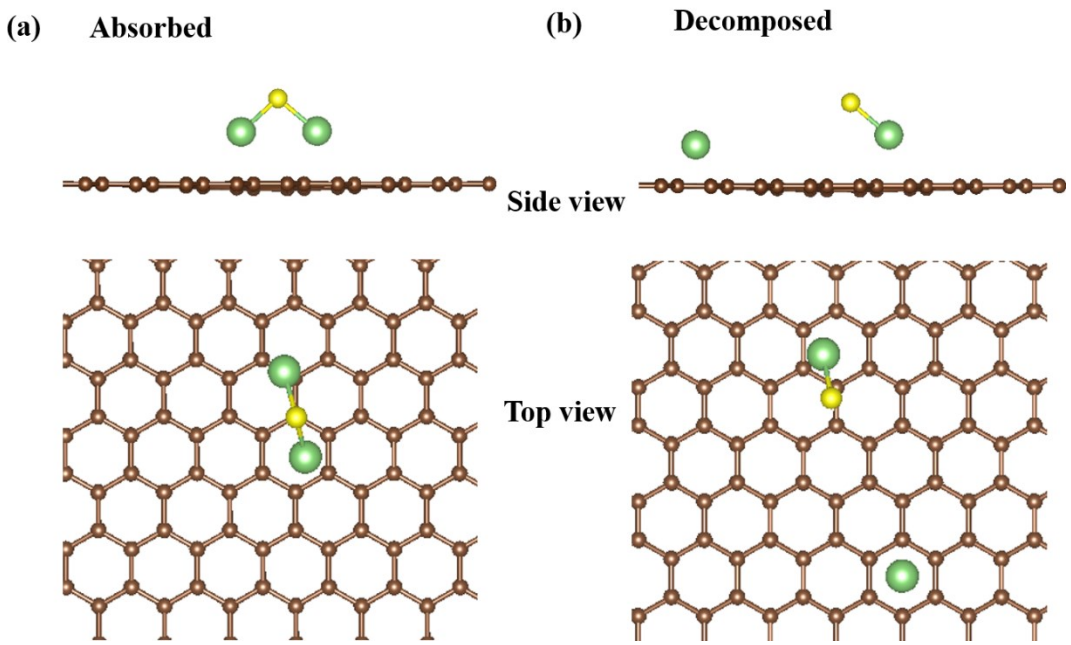


**Fig. S11** The calculated delithiation models of $Li_2S$ on HCPC surface in the (a) initially adsorbed and (b) decomposed structure.

Table S1 Electrochemical parameters derived from Tafel plots

| Samples | Tafel slop ($mV\ dec^{-1}$) | Exchange current density ($mA\ cm^{-2}$) |
|---|---|---|
| WCNP@HCPC-S | 19.3 | 0.29 |
| WCB@HCPC-S | 26.5 | 0.20 |
| HCPC-S | 52.4 | 0.13 |

Table S2 Comparison of adsorption energy and delithiation energy barriers

| Samples | Adsorption energy (eV) | Delithiation energy barriers (eV) |
|---|---|---|
| HCPC | -0.64 | 2.14 |
| WC (0001) | -5.82 | 0.10 |
| WC ($10\bar{1}0$) | -5.69 | 0.06 |