Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.


Supporting information

# Cobalt-doped tin disulfide catalysts for high-capacity lithium-air batteries with high lifetime

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Catalogue:

1. Experimental preparation

2. Calculation of DFT

3. Analysis of experimental and DFT results

## 1. Experimental preparation

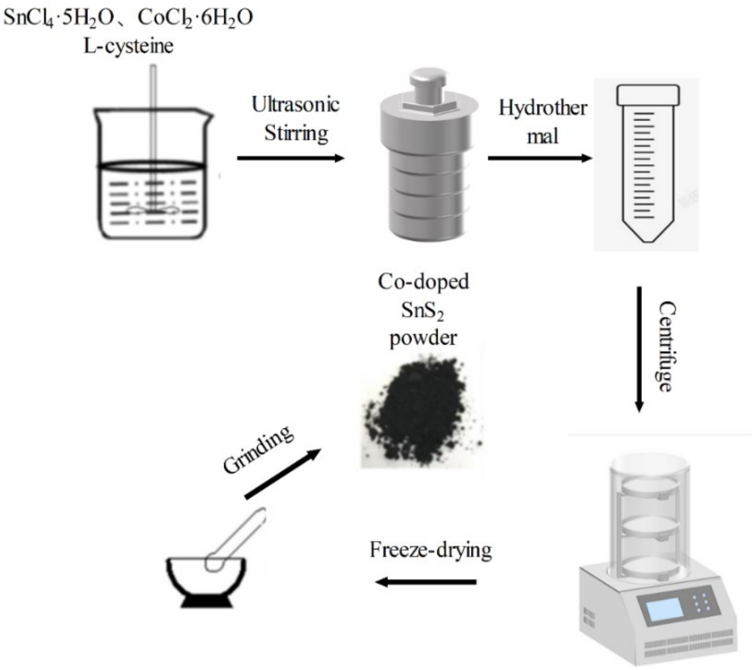


Fig. S1: Co-doped SnS2 preparation process

Table S1: Inventory of chemicals

| Name | Purity | Manufacturer |
|---|---|---|
| $SnCl_4·5H_2O$ | 99.8% | Shanghai Aladdin Biochemical Technology Co., Ltd. |
| $CoCl_2·6H_2O$ | 99.99% | Shanghai Aladdin Biochemical Technology Co., Ltd. |
| L-cysteine | 99.9% | Shanghai Aladdin Biochemical Technology Co., Ltd. |
| CNT | 99.9% | |
| LiOH | 95% | Sinopharm Group |
| PTFE | | Sinopharm Group |
| N-Methyl-pyrrolidone | AR | Sinopharm Group |
| Toray Carbon 060 Hydrophilic | | Suzhou Shengeruo Technology Co. |
| LISICON | | Shenzhen Kejing Star Technology Co |
| LITFSI-TEGDME | | NJ Scientific |

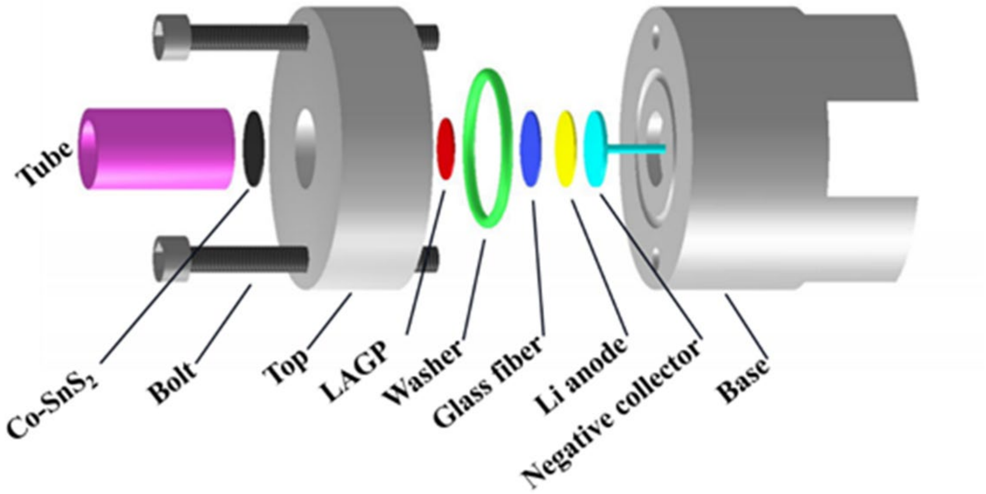


Fig. S2: Dual electrolyte lithium-air battery mould.

**2. Calculation of DFT**

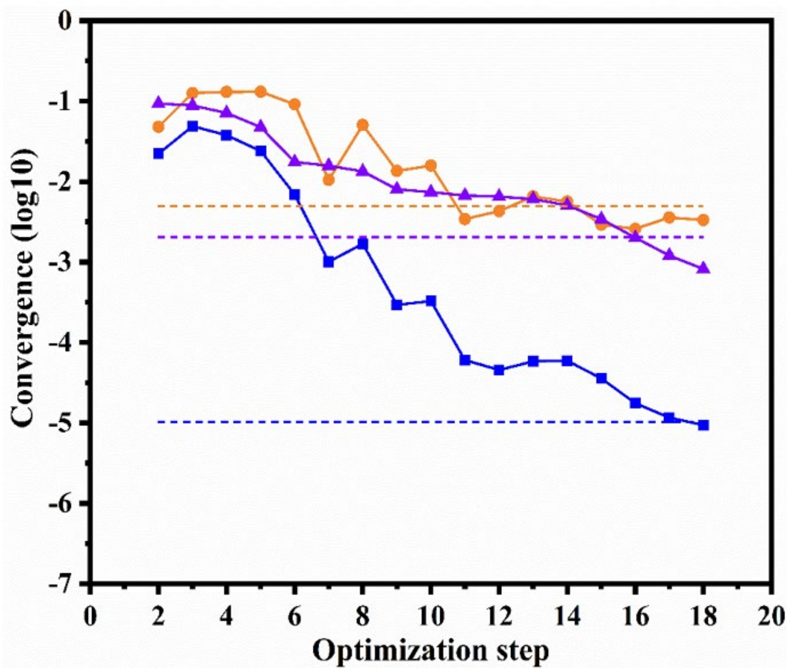


Figure. S3: Convergence curves.

Under alkaline conditions: ORR and OER four-electron reaction pathway:

ORR processes in alkaline environments:

$$O_2(g)+4e^-+2H_2O(l)\rightarrow 4OH^- \qquad S(1)$$

ORR process four-electron pathway:

$$O_2(g)+H_2O(l)+e^-+*\rightarrow OOH^*+OH^- \qquad (1)$$

$$OOH^*+e^-\rightarrow O^*+OH^- \qquad (2)$$

$$O^*+H_2O(l)+e^-\rightarrow OH^-+OH^* \qquad (3)$$

$$OH^*+e^-\rightarrow OH^-+* \qquad (4)$$

The OER process is the inverse of the ORR process:

$$4OH^-\rightarrow O_2(g)+4e^-+2H_2O \qquad S(2)$$

OER process four-electron pathway:

$$OH^-+*\rightarrow OH^*+e^- \qquad (1)$$

$$OH^-+OH^*\rightarrow O^*+H_2O(l)+e^- \qquad (2)$$

$$O^*+OH^-\rightarrow OOH^*+e^- \qquad (3)$$

$$OOH^*+OH^-\rightarrow O_2(g)+H_2O(l)+e^-+* \qquad (4)$$

where ＊ represents the base low, l represents the liquid phase and g represents the gas phase.

**3. Analysis of experimental and DFT results**

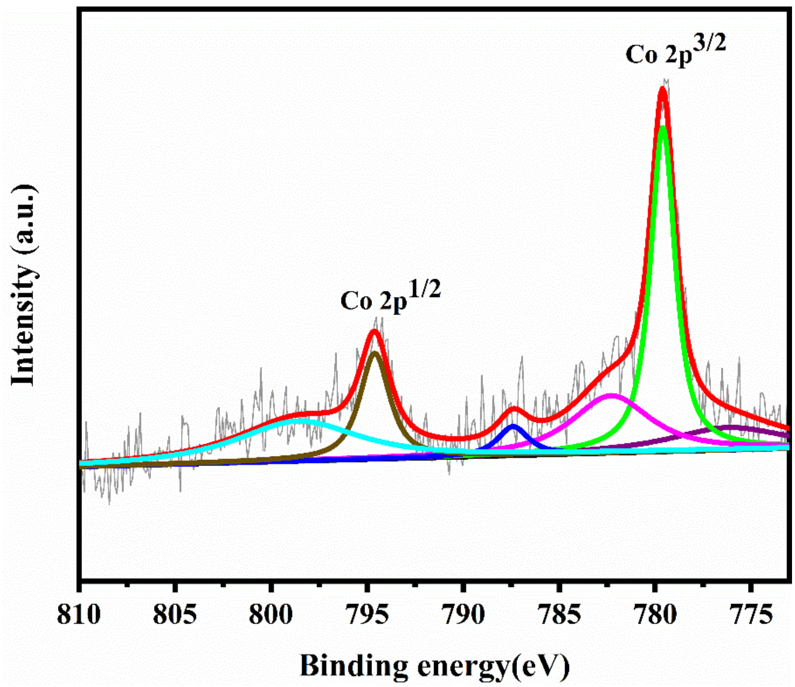


Fig. S4: Co2p spectrum

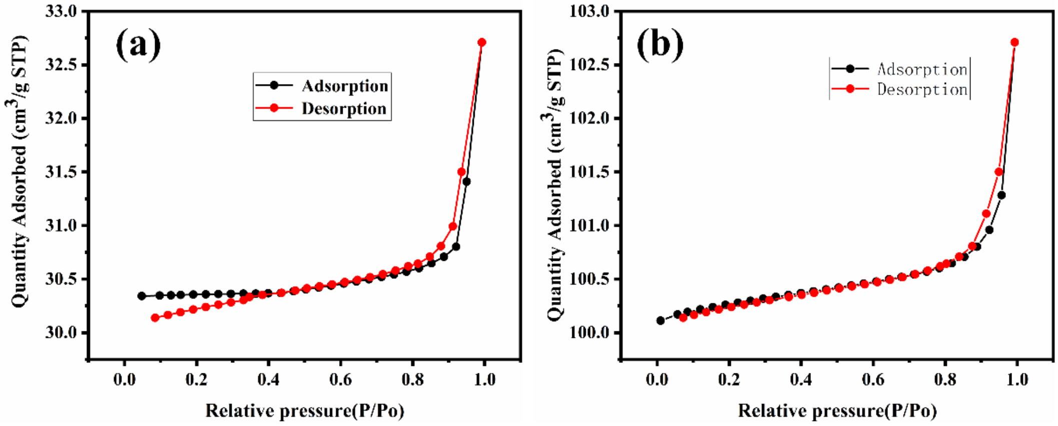


Figure.S5: (a) (b) Nitrogen adsorption and desorption isothermal curves for 0.02 Co-SnS2 pure SnS2 material, respectively.

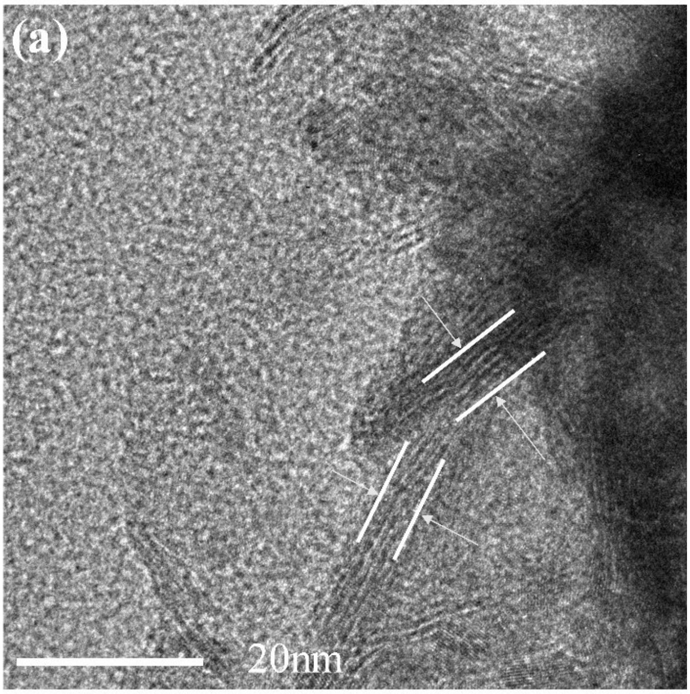


Fig. S6: Co-SnS2 HRTEM image.

Table S2: Conductivity measurement

| | $SnS_2$ | 0.01Co-$SnS_2$ | 0.02Co-$SnS_2$ | 0.04Co-$SnS_2$ |
|---|---|---|---|---|
| **Electrical conductivity** | 86.96s/cm | 105.7s/cm | 108.6s/cm | 101.1s/cm |

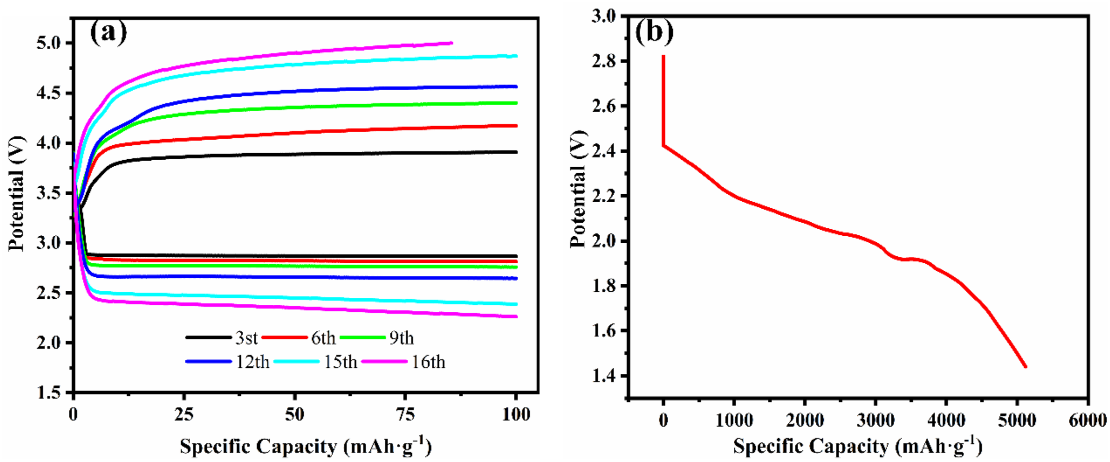


Fig. S7: (a) pure Co cycle performance, (b) maximum discharge capacity.

Table S3: Adsorbed $O_2$ bond lengths.

| | **1Co-$SnS_2$** | **2Co-$SnS_2$** | **3Co-$SnS_2$** |
|---|---|---|---|
| **$O_2$ 键长** | 1.226Å | 3.25 Å | 3.786 Å |

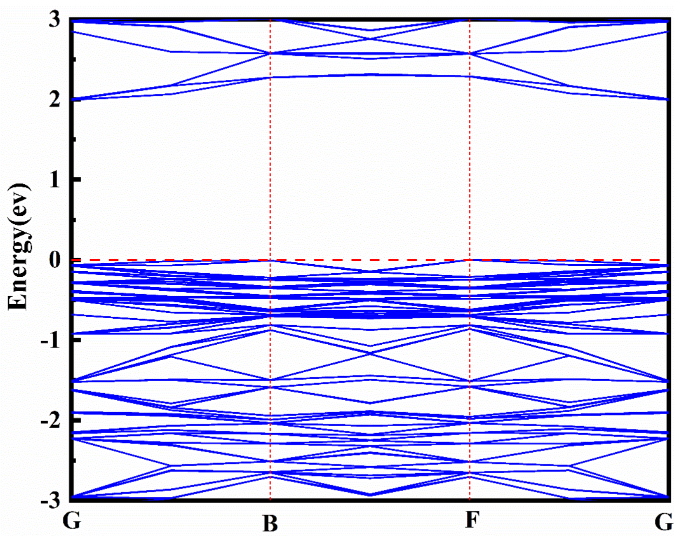


Fig. S8: SnS2 energy band diagram.

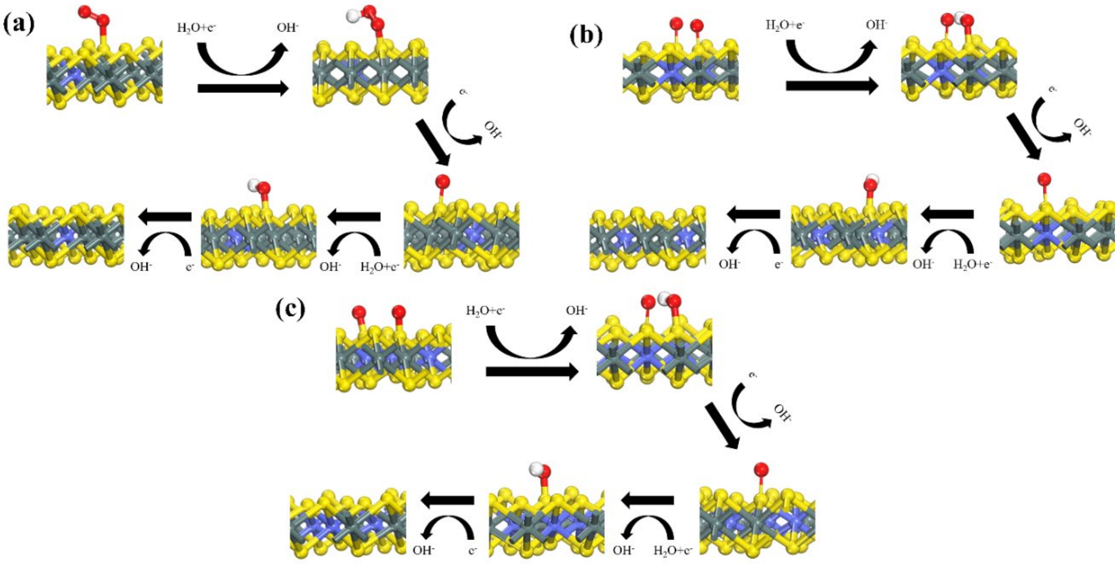


Fig. S9: (a) 1Co-Sn, (b) 2Co-Sn, (c) 3Co-Sn redox schematic.

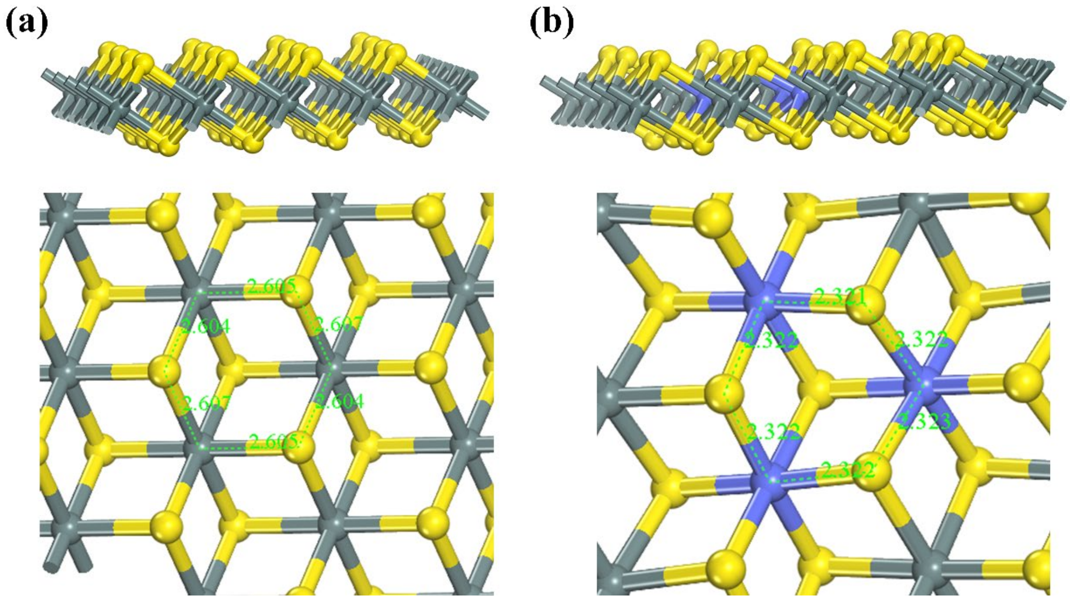


Fig. S10 (a) SnS2 model, (b) 3Co-Sn model.

Table S4: Comparison of battery performance.

| Catalyst | Cycling number | Initial discharge Capacity(mAh·g$^{-1}$) | Overpotential(V) | Ref |
|---|---|---|---|---|
| Co-doped $SnS_2$ | 132(528h) | 16065 | 0.7 | This work |
| Boron doped CNT | 165(330h) | 8900 | 0.3 | Wang[1] |
| MNO-CNT-CNFFs | 21(120h) | | 0.15(low current) | Ji[2] |
| N doped GNSs | | | 0.88 | Yoo[3] |
| N-MC + NCONF@Ni | 100(400h) | | | Li[4] |

**Reference**


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