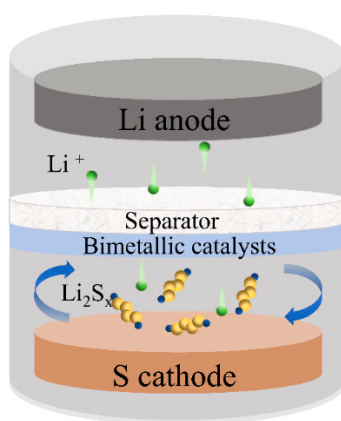


## Supporting Information

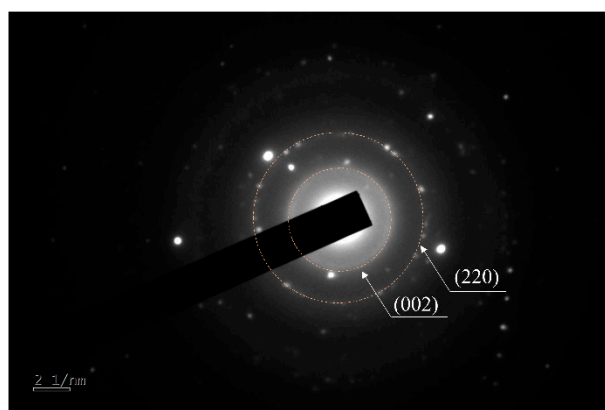
### Optimized *d* orbital electronic structure by constructing bimetallic compounds for catalytic effect of lithium-sulfur batteries

Liping Chen, Runhua Wang, Nan Li, Yang Bai, Yimo Zhou, Yonghong Fu, Juan Wang\*

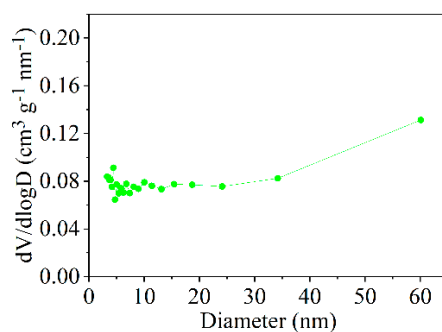
Shaanxi Key Laboratory of Nanomaterials and Nanotechnology, Xi'an Key Laboratory of Clean Energy, Xi'an University of Architecture and Technology, Xi'an 710055, P.R. China



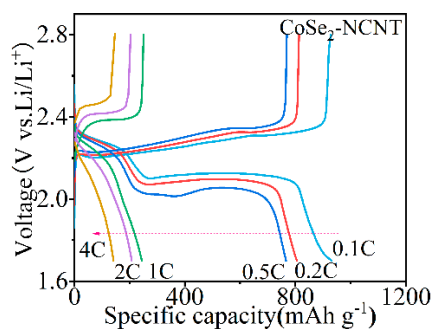
**FigureS1.** Scheme of Li-S battery with modified separator



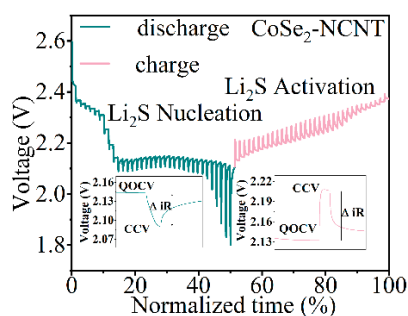
**Figure S2.** Selected area electron diffraction (SAED) pattern of  $(\text{Cu},\text{Co})\text{Se}_2$



**FigureS3.** Pore size distribution of CoSe<sub>2</sub>-NCNT



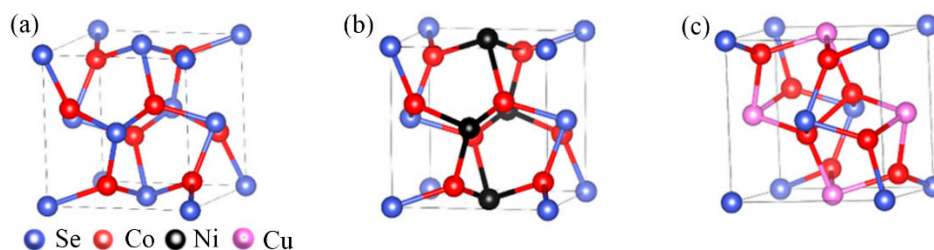
**FigureS4.** Charge-discharge curves of battery with CoSe<sub>2</sub>-NCNT at different rate



**FigureS5.** GITT plots of Li-S batteries with CoSe<sub>2</sub>-NCNT

$$\Delta R_{\text{intern}}(\Omega) = |\Delta V_{\text{QOCV-CCV}}| / I_{\text{applied}} \quad \text{S(1)}$$

where  $\Delta R_{\text{intern}}(\Omega)$  refers to the internal resistances of Li-S batteries, QOCV and CCV are the quasi-open-circuit voltage and closed-circuit-voltage, respectively. And the  $\Delta V_{\text{QOCV-CCV}}$  represents their difference,  $I_{\text{applied}}$  stands for the applied current.



**FigureS6.** Theoretical calculation structure model of (a) CoSe<sub>2</sub>, (b) (Ni,Co)Se<sub>2</sub>, (c) (Cu,Co)Se<sub>2</sub>

Table S1 The content of each element in (CuCo)Se<sub>2</sub>

Elements	wt. %	at. %
C	35.88	73.83
N	3.15	5.55
Co	10.02	4.20
Cu	6.23	2.42
Se	44.72	14.00

Table S2 Comparison of electrochemical performance of Li-S batteries with different catalysts

Samples	Specific capacity (mAh g <sup>-1</sup> )			Capacity decay rate	$\Delta E$ (mV)	
	0.1C	4C	1C	1C	2C	4C
CoSe <sub>2</sub>	814.81	142.18	657.44	0.084%	580	730
(NiCo)Se <sub>2</sub>	1410.41	395.68	838.63	0.123%	630	690
(CuCo)Se <sub>2</sub>	1670.08	838.27	1051.06	0.086%	360	600

Table S3 Theoretical model structural parameters of different materials

	Lattice A	Lattice B	Lattice C
CoSe <sub>2</sub>	5.848	5.848	5.848
(Ni,Co)Se <sub>2</sub>	5.900	5.886	5.883
(Cu,Co)Se <sub>2</sub>	6.043	5.954	5.954

Table S4 *d* orbital electronic structure parameters of different (MCo)Se<sub>2</sub>

Materials	<i>d</i> band center (eV)		<i>d</i> orbital occupation number	
	Co	M	Co	M
CoSe <sub>2</sub>	-1.292	-	7.61	-
(NiCo)Se <sub>2</sub>	-1.070	-1.461	7.43	8.75
(CuCo)Se <sub>2</sub>	-1.314	-2.403	7.98	9.03