

Supplementary Materials

Ni-doped CoTe with optimized *p*-band center for boosting polysulfide conversion kinetics in lithium-sulfur batteries

Jingjing Qie^{1,#}, Huiyue Sun^{1,#}, Shuang Geng^{1,#}, Yongqi Shang¹, Qunzhi Huang¹, Jishi Wei^{1,2,*}, Ke Chen¹, Taifeng Liu³, Shuxi Dai^{1,*}, Wuxing Hua^{1,4,*}, Zhen Zhou⁴

¹Center for the Physics of Low-Dimensional Materials, Henan Joint International Research Laboratory of New Energy Materials and Devices, School of Physics and Electronics, Henan University, Kaifeng 475004, Henan, China.

²Henan Key Laboratory of Protection and Safety Energy Storage of Light Metal Materials, College of Chemistry and Molecular Sciences, Henan University, Kaifeng 475004, Henan, China.

³National & Local Joint Engineering Research Center for Applied Technology of Hybrid Nanomaterials, Henan University, Kaifeng 475004, Henan, China.

⁴College of New Energy and Intelligent Manufacturing, National Key Laboratory of Green Chemical Synthesis and Transformation Technology, Henan University, Zhengzhou 450046, Henan, China.

[#]These authors contributed equally to this work.

***Correspondence to:** Prof. Jishi Wei, Prof. Shuxi Dai, Prof. Wuxing Hua, Center for the Physics of Low-Dimensional Materials, Henan Joint International Research Laboratory of New Energy Materials and Devices, School of Physics and Electronics, Henan University, Kaifeng 475004, Henan, China. E-mail: ecjsw@henu.edu.cn; shuxidai@henu.edu.cn; wxhua@henu.edu.cn

Supporting Figures and Tables

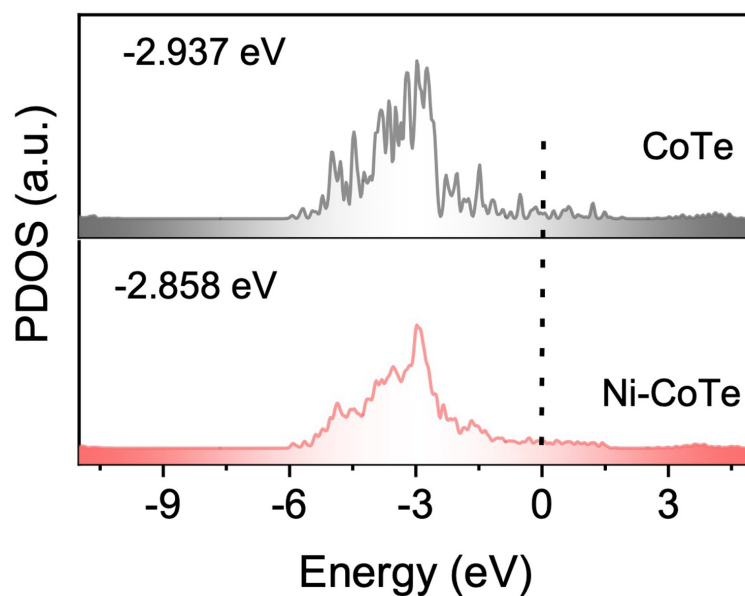


Figure S1. PDOS of d orbitals and corresponding d -band centers for CoTe doped with Ni.

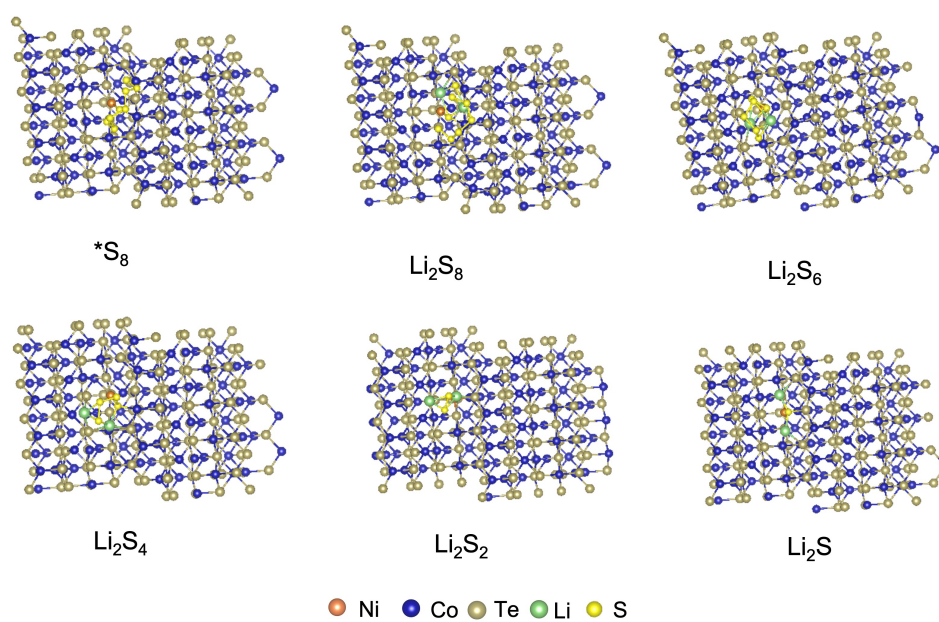


Figure S2. Adsorption configurations of S_8 and Li_2S_x ($x = 1, 2, 4, 6, 8$) on Ni-CoTe.

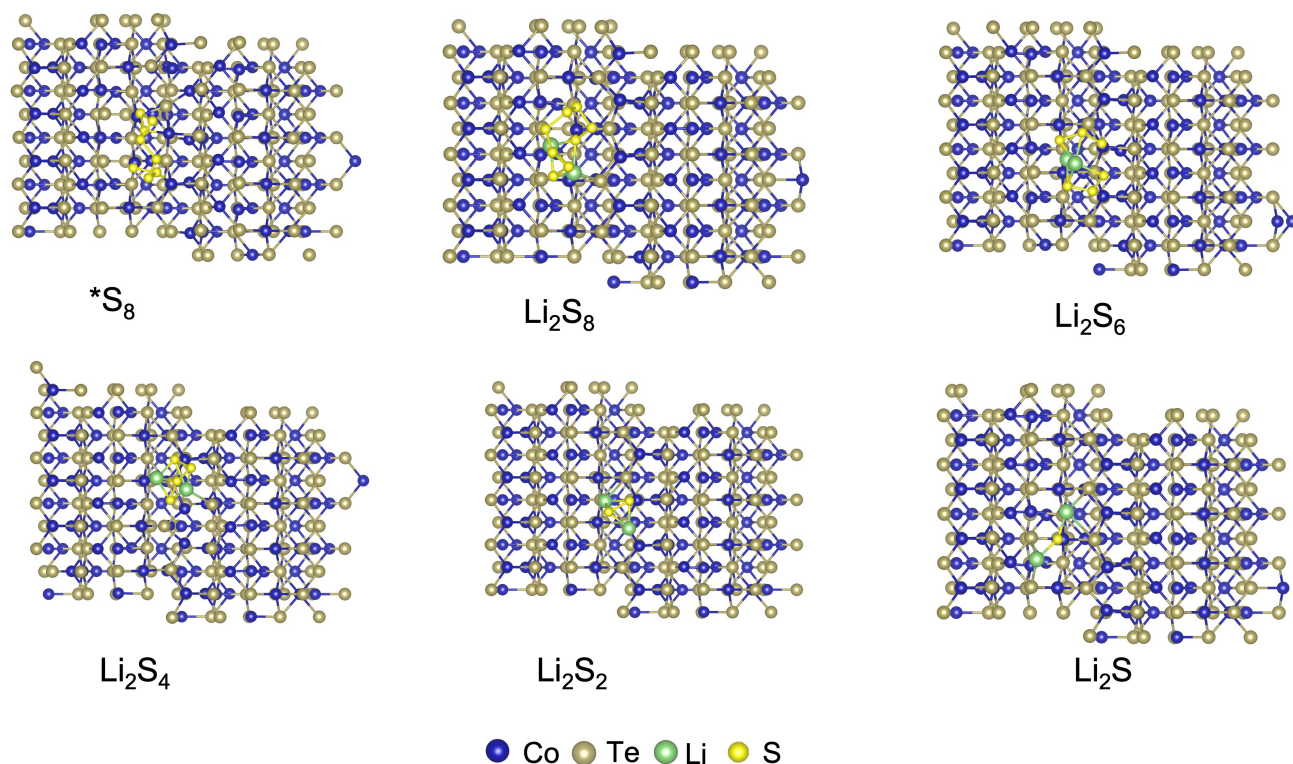


Figure S3. Adsorption configurations of S_8 and Li_2S_x ($x = 1, 2, 4, 6, 8$) on CoTe.

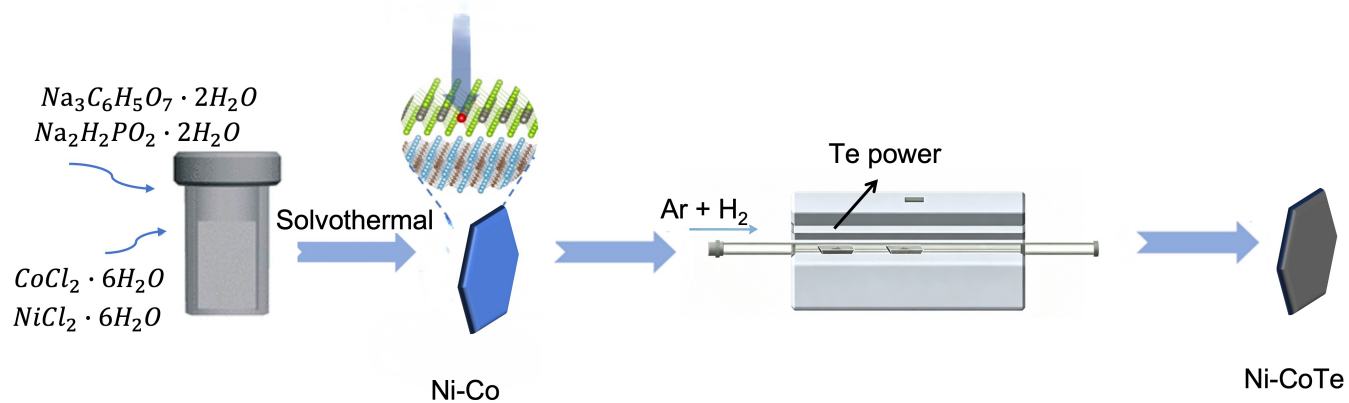


Figure S4. Schematic illustration of the synthesis procedure for Ni-CoTe.

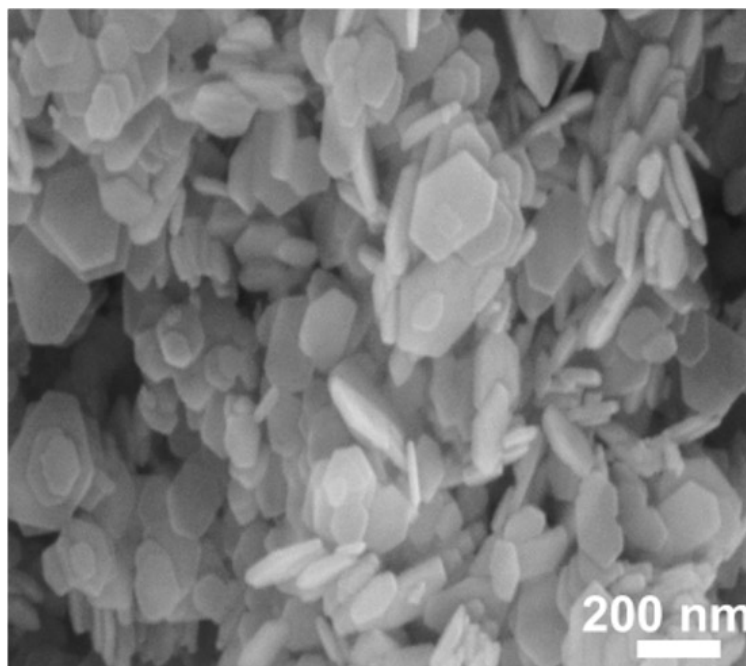


Figure S5. SEM images of the Ni-Co nanosheets.

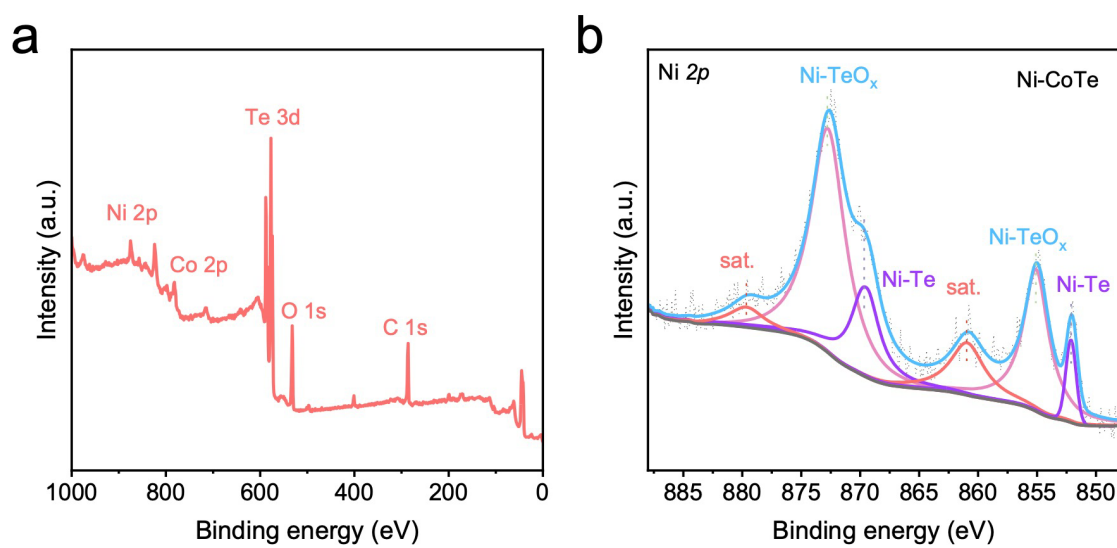


Figure S6. (a) XPS survey spectra of Ni-CoTe. (b) XPS spectra of Ni 2p in Ni-CoTe.

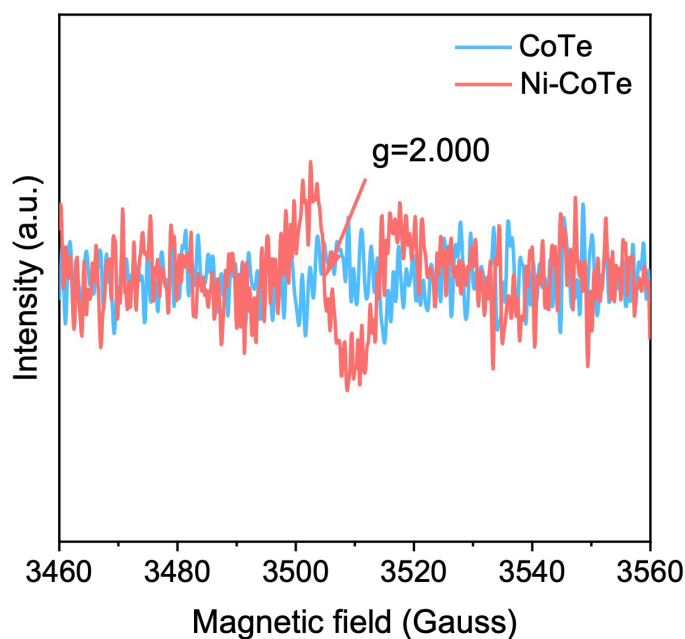


Figure S7. EPR spectra of the Ni-CoTe and CoTe catalysts.

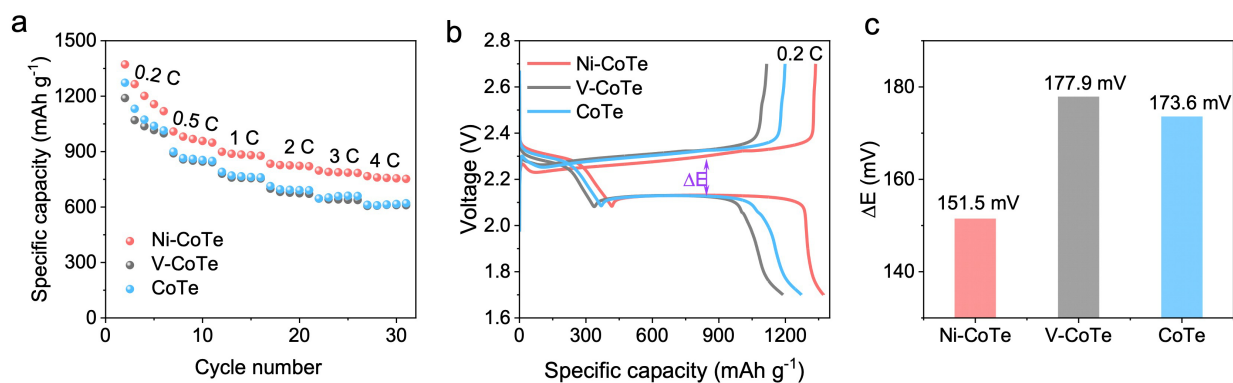


Figure S8. (a) Rate performance of Ni-CoTe, V-CoTe, and CoTe batteries from 0.2 to 4 C. (b) Galvanostatic discharge-charge profiles of the three batteries at 0.2 C. (c) Overpotentials derived from the voltage difference between charge and discharge plateaus at 0.2 C.

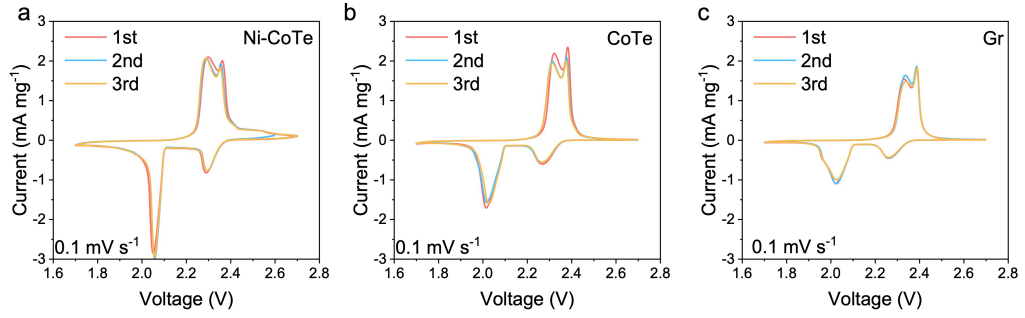


Figure S9. Three consecutive CV curves of Ni-CoTe, CoTe and Gr batteries at a scan rate of 0.1 mV s^{-1} .

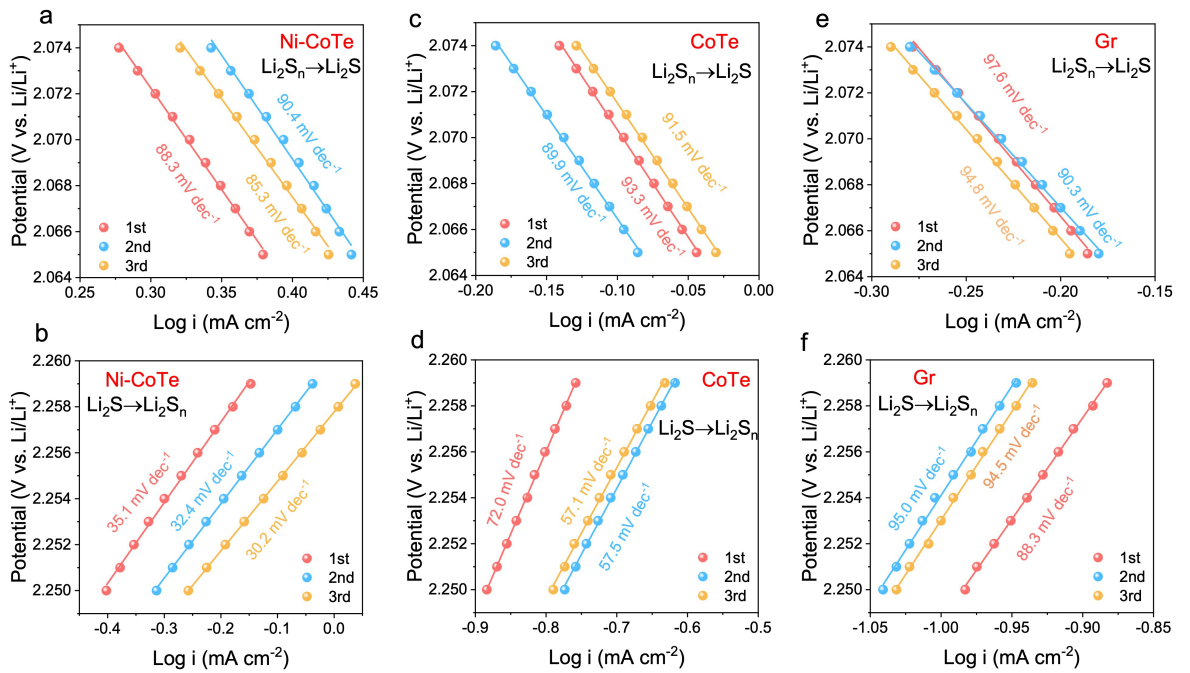


Figure S10. The Tafel plots for Ni-CoTe, CoTe, and Gr batteries were obtained by fitting data from three consecutive CV cycles.

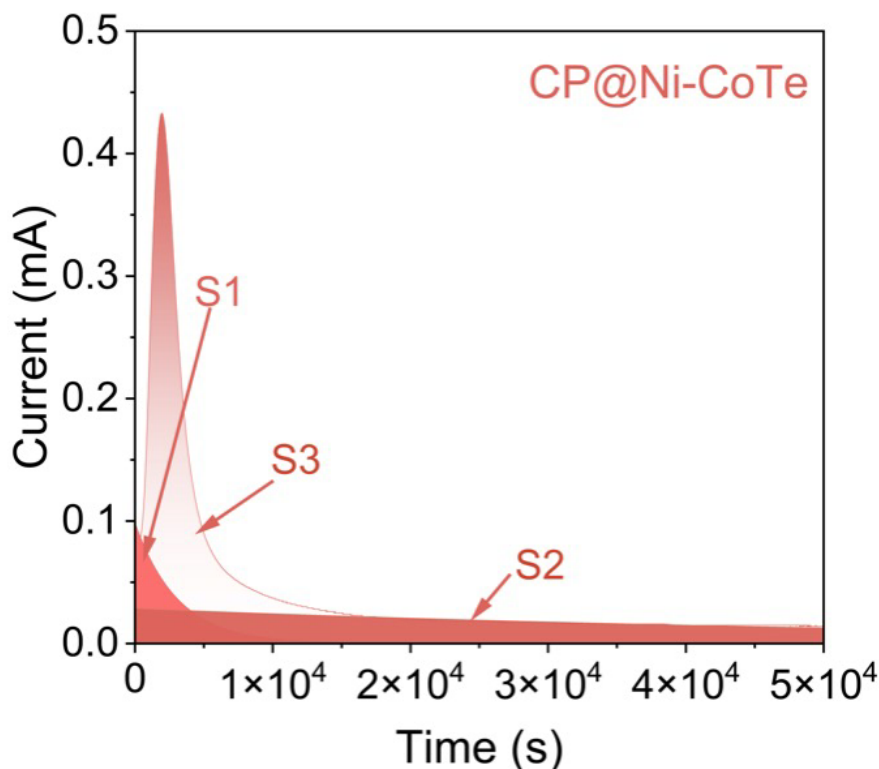


Figure S11. Potentiostatic discharge profiles at 2.05 V on Ni-CoTe catalyst.

To investigate the Li_2S deposition process, the CP@Ni-CoTe cell was first discharged galvanostatically to 2.06 V, followed by a potentiostatic discharge at 2.05 V, during which Li_2S began to precipitate." The area under the potentiostatic discharge curves in Figure S11 could be mathematically modeled as three parts (S1, S2, S3): S1 and S2 correspond to the sequential reductions of Li_2S_8 and Li_2S_6 , respectively, while S3 is attributed to the precipitation of Li_2S ^{1, 2}. The corresponding conversion capacity was quantitatively determined based on Faraday's law. Specifically, denoting the total integral area of the potentiostatic curve as S0, and the weight of sulfur in the Li_2S_8 electrolyte is denoted as W, the specific capacity for Li_2S precipitation was calculated as $(S0 - S1 - S2) / (3600 \times W)$.

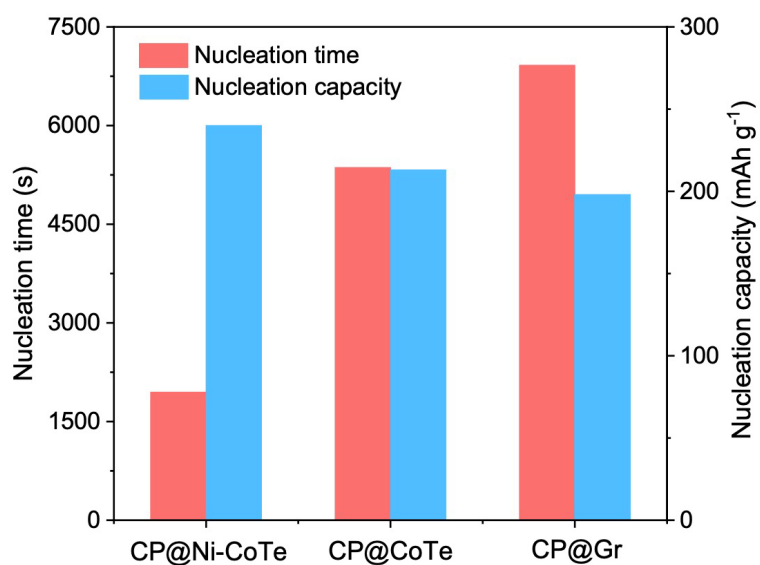


Figure S12. Bar chart of Li₂S nucleation time and nucleation capacity.

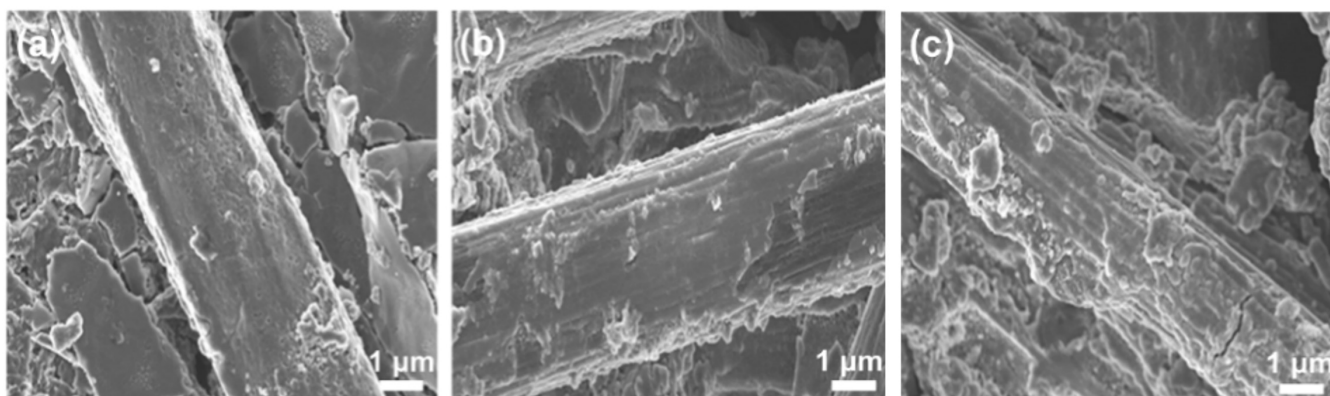


Figure S13. SEM images of (a) CP@Ni-CoTe, (b) CP@CoTe, and (c) CP@Gr after Li₂S deposition.

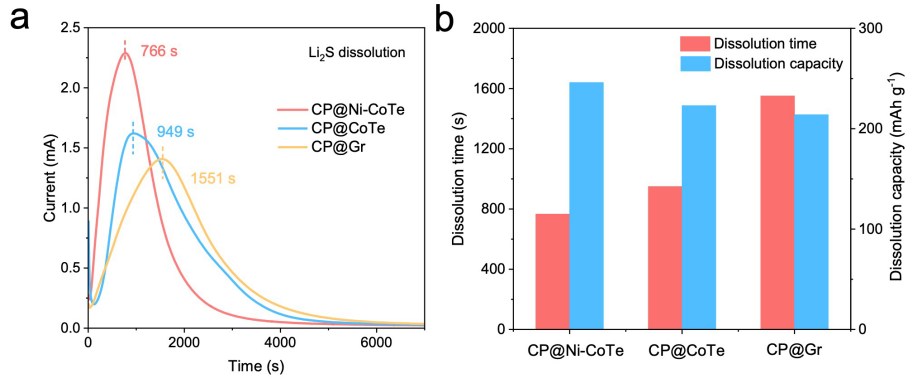


Figure S14. (a) Potentiostatic current-time profiles for Li_2S oxidation and dissolution on CP@Ni-CoTe, CP@CoTe, and CP@Gr substrates. (b) Corresponding Li_2S dissolution capacities and dissolution times derived from the potentiostatic measurements.

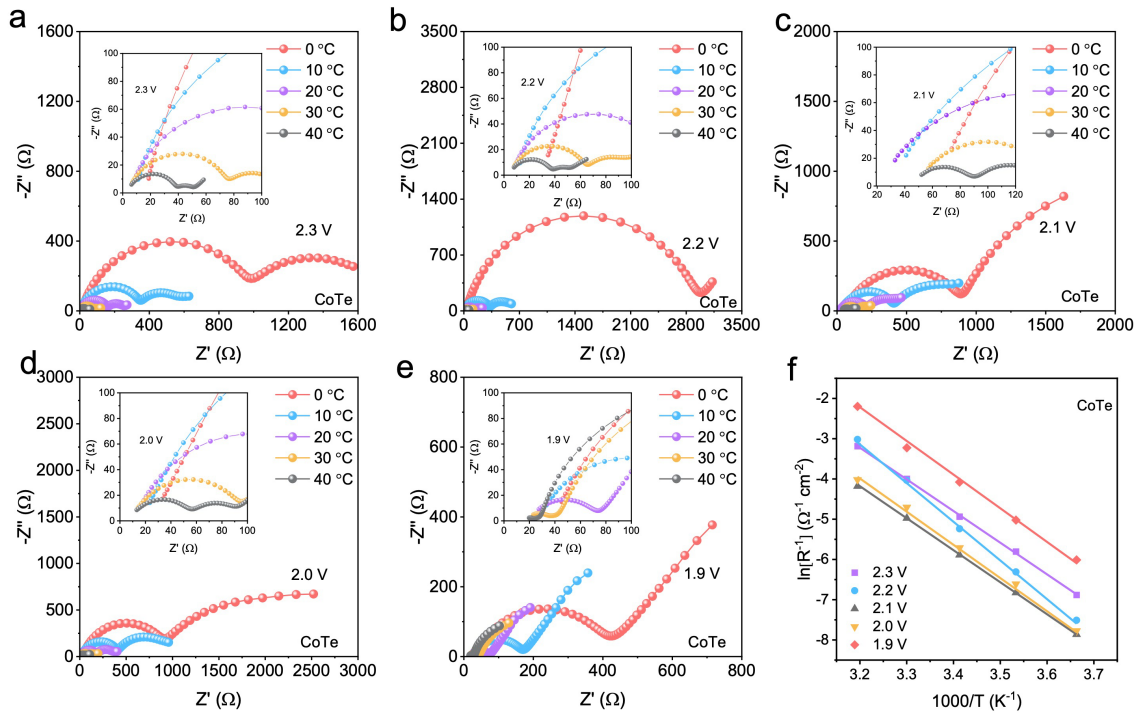


Figure S15. (a-e) EIS measurements of the CoTe battery at various temperatures at 1.9-2.3 V, revealing the reaction kinetics during the discharge process. (f) Arrhenius plots for the CoTe battery calculated from the EIS curves.

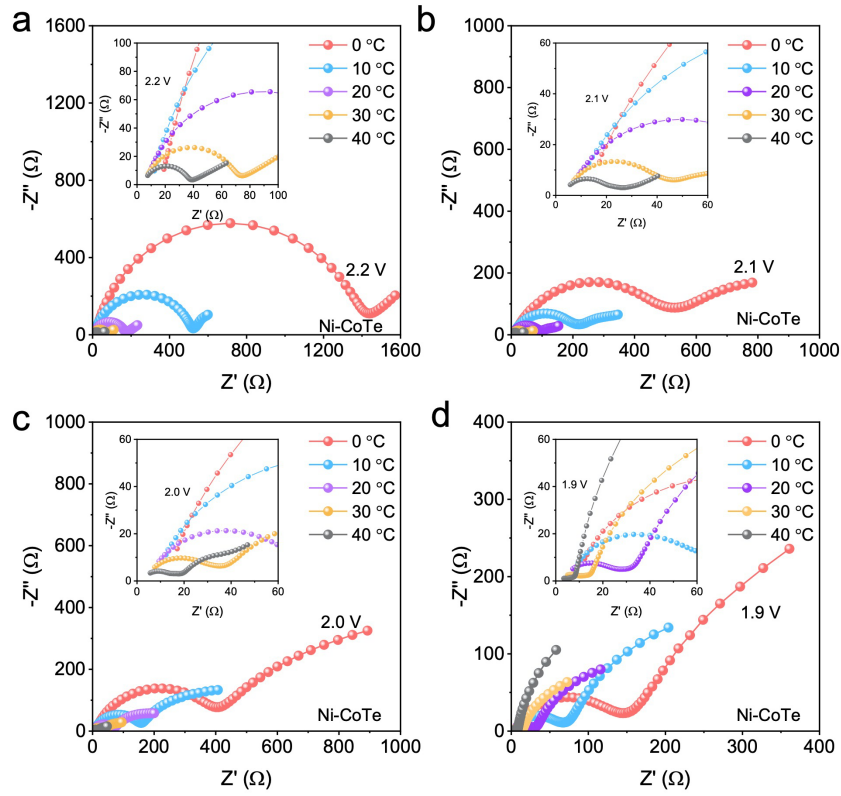


Figure S16. (a-d) EIS measurements of the Ni-CoTe battery at various temperatures at 1.9-2.2 V, revealing the reaction kinetics during the discharge process.

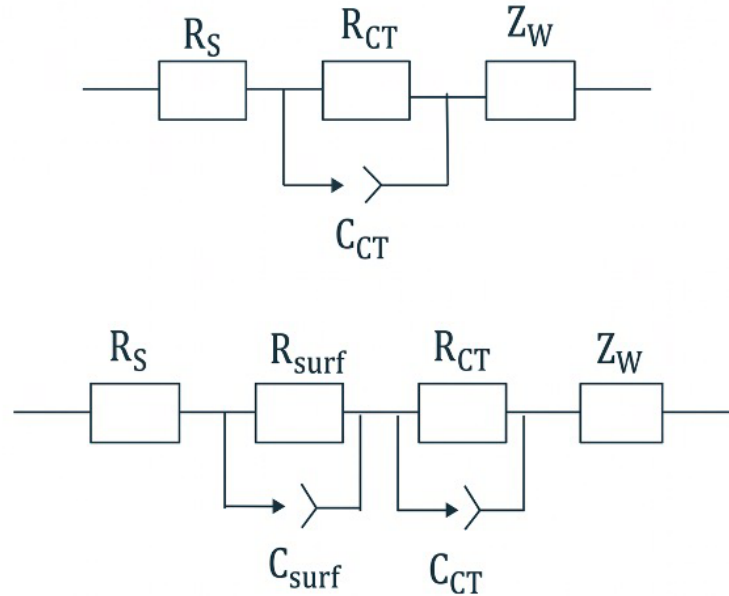


Figure S17. Simplified-contact Randles-equivalent circuits of EIS in Supplementary Figures S15-16.

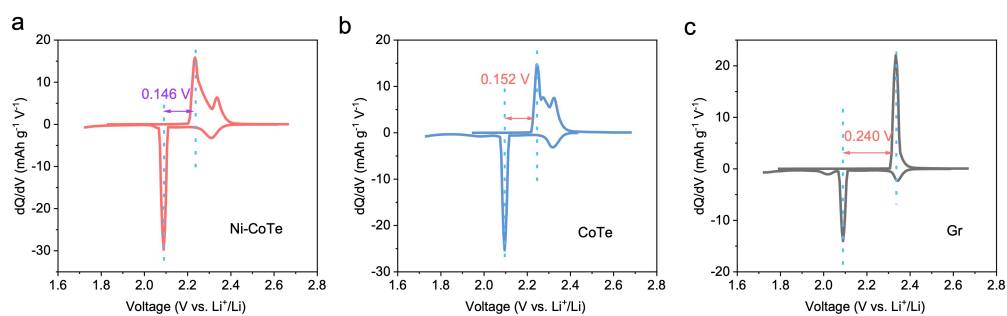


Figure S18. The differential plots corresponding to the charge/discharge profiles of Ni-CoTe, CoTe, and Gr batteries in Figure 4b.

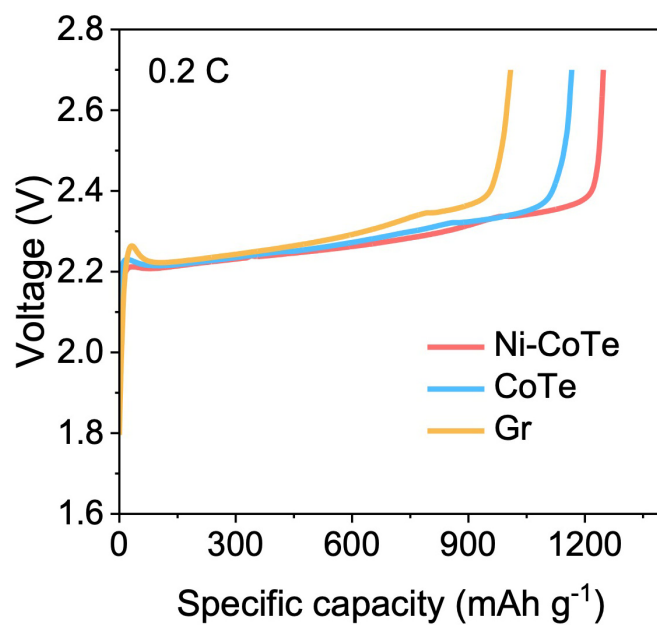


Figure S19. Charge profiles in the second cycle of the three batteries at 0.2 C.

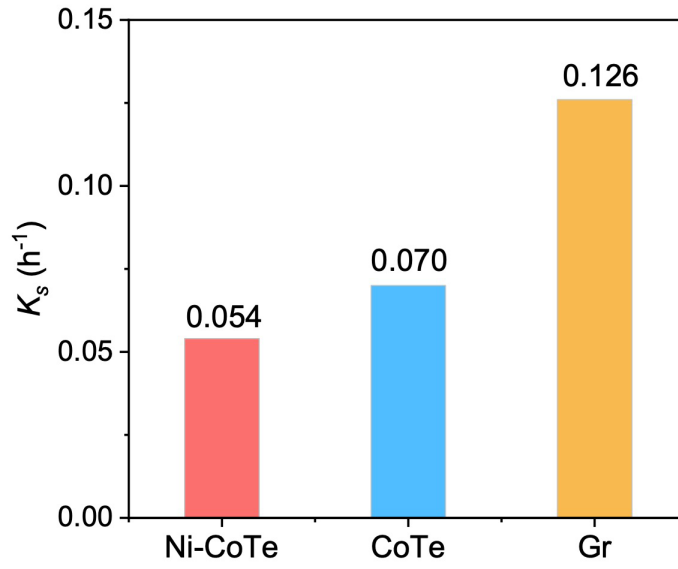


Figure S20. Shuttle constants of the Ni-CoTe, CoTe, and Gr batteries.

The shuttle constants (k_s , h^{-1}) were derived from the initial discharge curves (Figure 4b) and the second charge curves (Figure S19) of the Ni-CoTe, CoTe, and Gr batteries at 0.2 C using the following formulae³:

$$\frac{k_s q_H [S_{total}]}{I_C} = f_C \quad (1)$$

$$H_{OC} = \frac{Q_H^{applied} - Q_H^{acc}}{Q_H^{acc}} = -\frac{1}{f_C} \ln(1 - f_C) - 1 \quad (2)$$

Where f_C is the charge-shuttle factor; $[S_{total}]$ is the total sulfur mass in the battery; q_H is the high plateau capacity (419 mAh g^{-1}); I_C is the current density at 0.2 C; $Q_H^{applied}$ is the applied high plateau charge capacity (taken as the maximum charge capacity); Q_H^{acc} is the high plateau accumulated charge capacity (taken as the practical charge capacity).

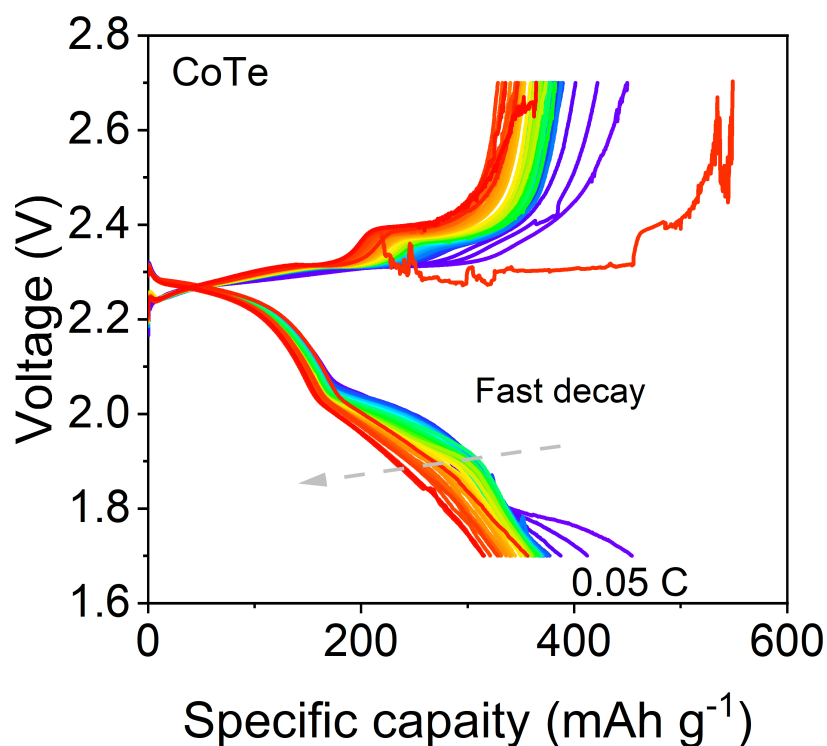


Figure S21. Galvanostatic charge-discharge profiles of CoTe batteries at 0.05 C.

Table S1. Comparison of cycle performance between Ni-CoTe and other modified separators reported in the literature

Modified materials	Sulfur loading (mg cm ⁻²)	Initial areal capacity (mAh cm ⁻²)	Reversible areal capacity (mAh cm ⁻²)	E/S ratio (μL mg ⁻¹)	Refs.
Ni-CoTe	10	13.5	8.4	5.0	This work
WNO-MCS@PP	8	7.7	7.1	8.3	4
Co/NbC@NC	6.5	4.8	4.3	5.9	5
Co-WO ₂	6.4	6.3	/	8.0	6
MoO ₃ /Co ₃ O ₄ @C	13.0	11.9	/	5	7
Bio-N-CNT	8.6	7.2	/	/	8
Co/MoN	4.92	4.6	2.7	10.0	9
NbS ₂	9.9	11.0	8.1	/	10

MoNQDs/NC	9.1	8.3	8.2	5.6	11
Co _{0.9} Zn _{0.1} Te ₂ @NC	7.7	12.8	7.9	4.0	12
Co ₃ O _{4-y} -CoO@rG	6.7	6.9	6.5	5.0	13

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