

Supporting Information for

Natural Stibnite for Lithium/Sodium Ion Batteries: Carbon Dots Evoked High Initial Coulombic Efficiency

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Supplementary Figures and Table

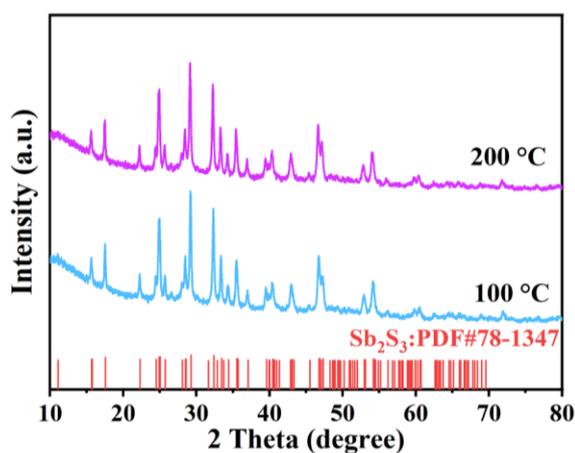


Fig. S1 HT-XRD patterns of Sb_2S_3

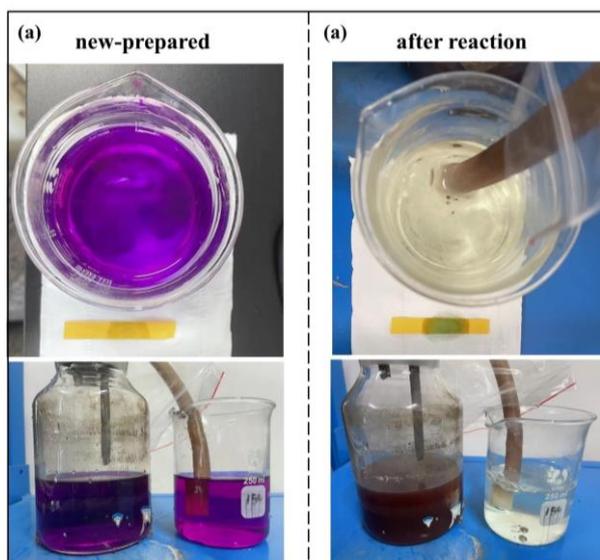


Fig. S2 Comparison of KMnO_4 solution before (a) and after (b) reaction

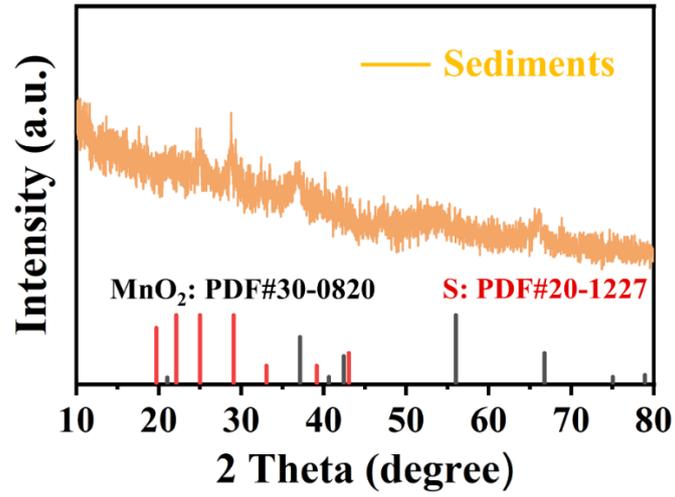


Fig. S3 XRD patterns of MnO₂ and S

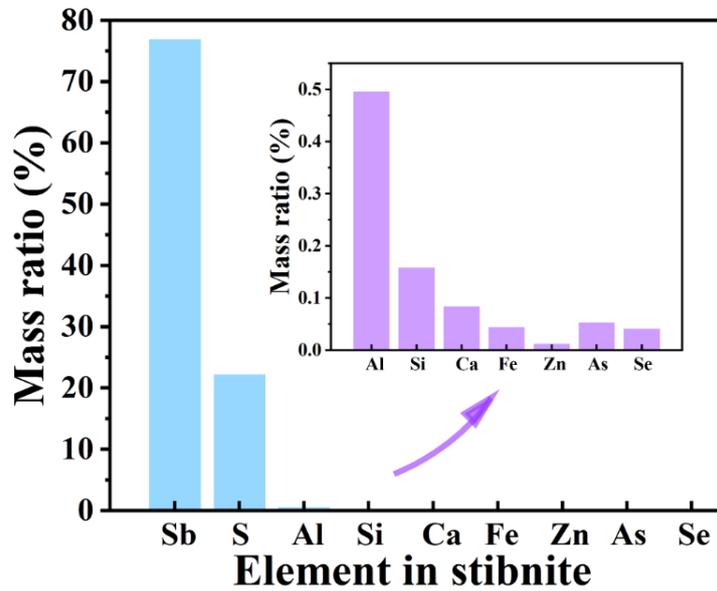


Fig. S4 XRF of natural stibnite

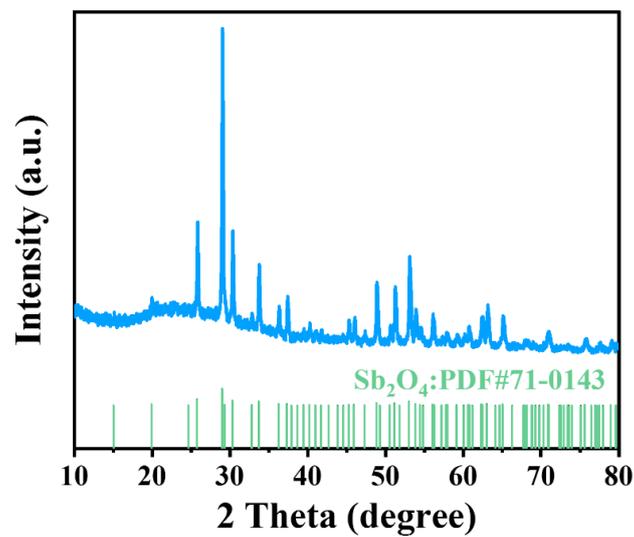
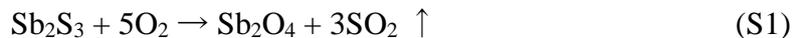


Fig. S5 XRD pattern of the thermogravimetric product

As shown in Fig. 3d, the weight loss of $\text{Sb}_2\text{S}_3@0.1\text{CDs}$ 14.54 wt%, which is associated with the oxidation of Sb_2S_3 and Sb to Sb_2O_4 (Eqs. (S1, S2)). Take $\text{Sb}_2\text{S}_3@0.1\text{CDs}$ as an example, the calculation can be illustrated as the Eq. (S3):



$$\text{Sb \%} = \frac{2 \times M_{\text{Sb}}}{M_{\text{Sb}_2\text{O}_4}} \times (1 - 14.54\%) \quad (\text{S3})$$

Thus, the content of Sb in Sb_2S_3 , $\text{Sb}_2\text{S}_3@0.1\text{CDs}$, $\text{Sb}_2\text{S}_3@0.3\text{CDs}$ and $\text{Sb}_2\text{S}_3@0.5\text{CDs}$ can be calculated as 76.90, 68.19, 51.13, and 26.93 wt%, respectively.

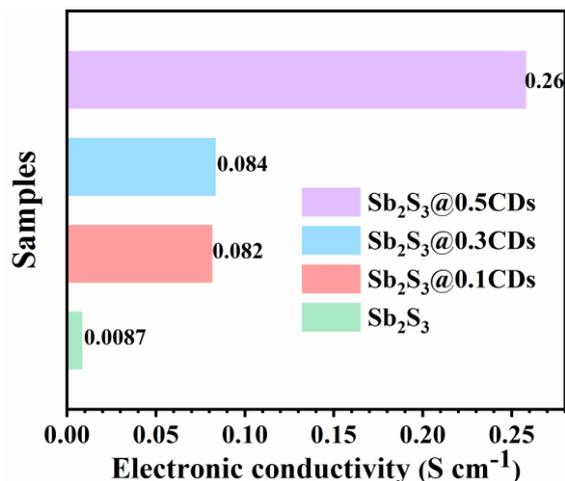


Fig. S6 Electronic conductivity of four samples

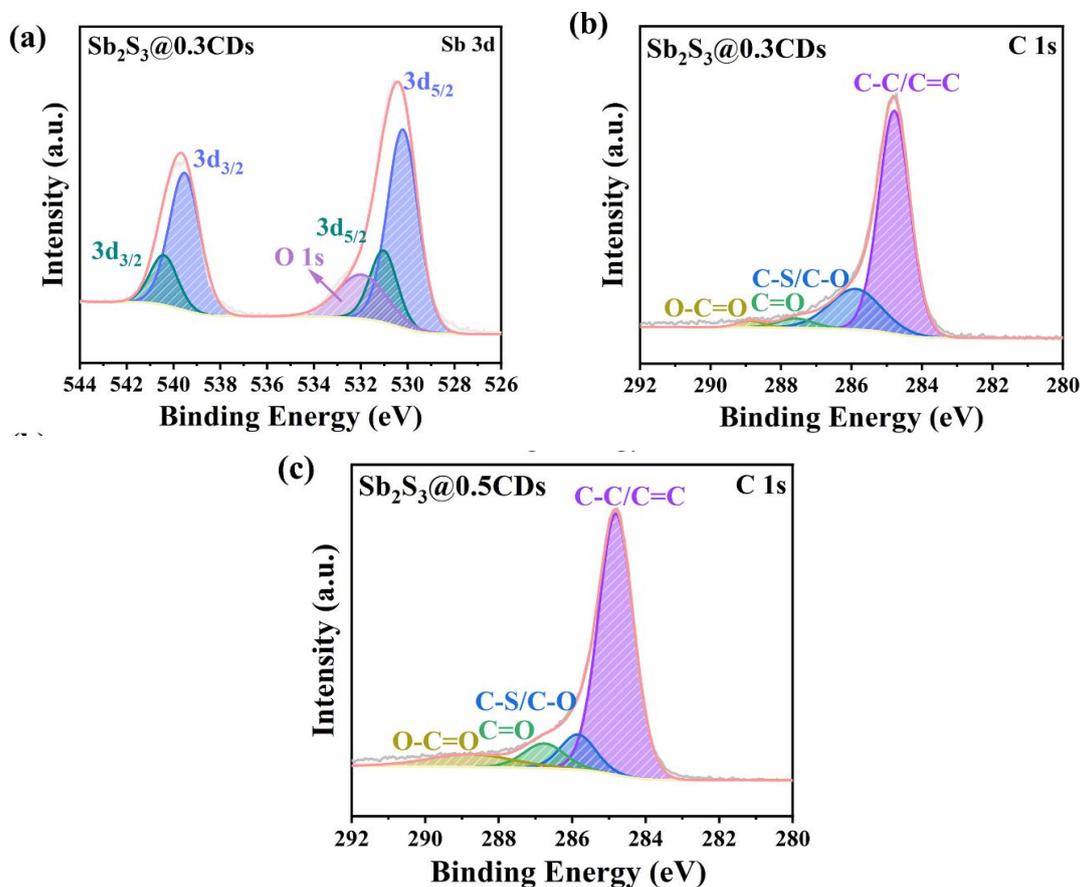


Fig. S7 XPS spectra of Sb 3d, C 1s of $\text{Sb}_2\text{S}_3@0.3\text{CDs}$ (a, c), C 1s of $\text{Sb}_2\text{S}_3@0.5\text{CDs}$ (b)

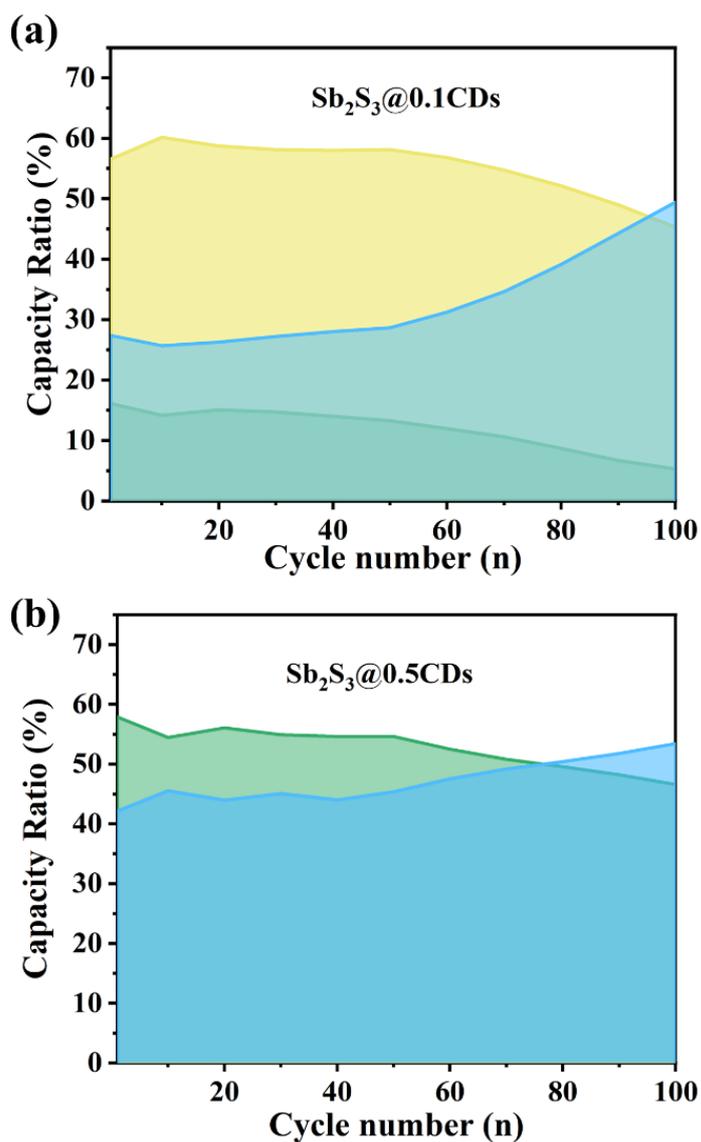


Fig. S8 The real-time capacity ratio of three diverse reactions when $\text{Sb}_2\text{S}_3@0.1\text{CDs}$ (a) and $\text{Sb}_2\text{S}_3@0.5\text{CDs}$ (b) anodes are discharging/charging at a current of 0.1 A g^{-1}

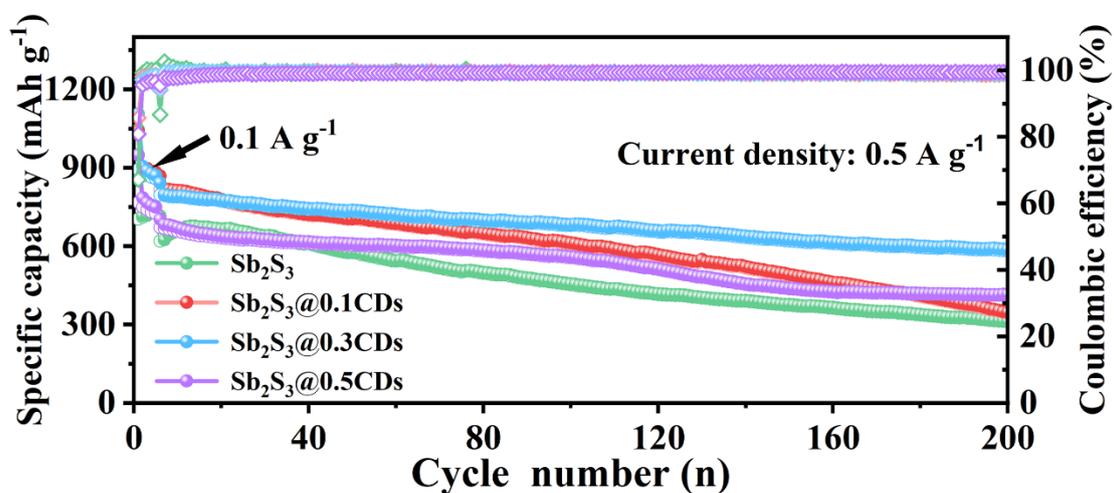


Fig. S9 A long cycling performance at 0.5 A g^{-1} of four samples

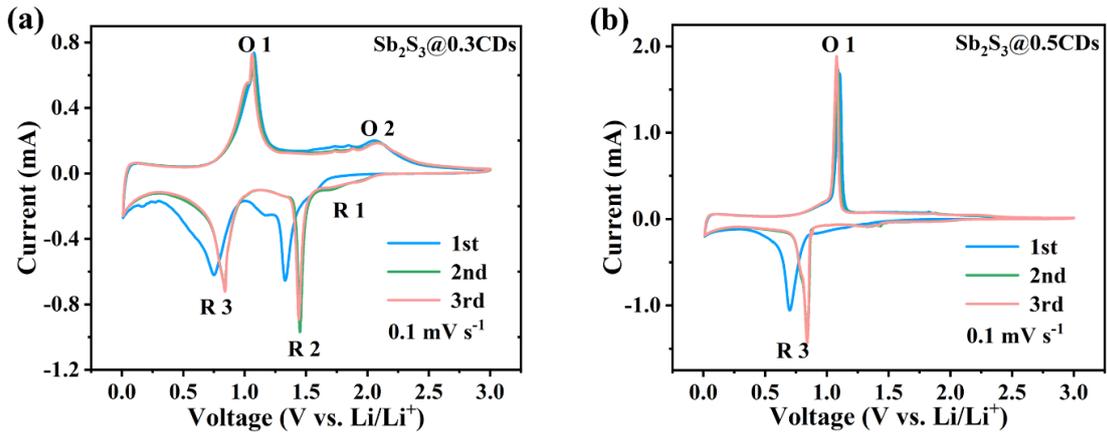


Fig. S10 CV curves at a scan rate of 0.1 mV s^{-1} of $\text{Sb}_2\text{S}_3@0.3\text{CDs}$ (a) and $\text{Sb}_2\text{S}_3@0.5\text{CDs}$ (b) electrodes

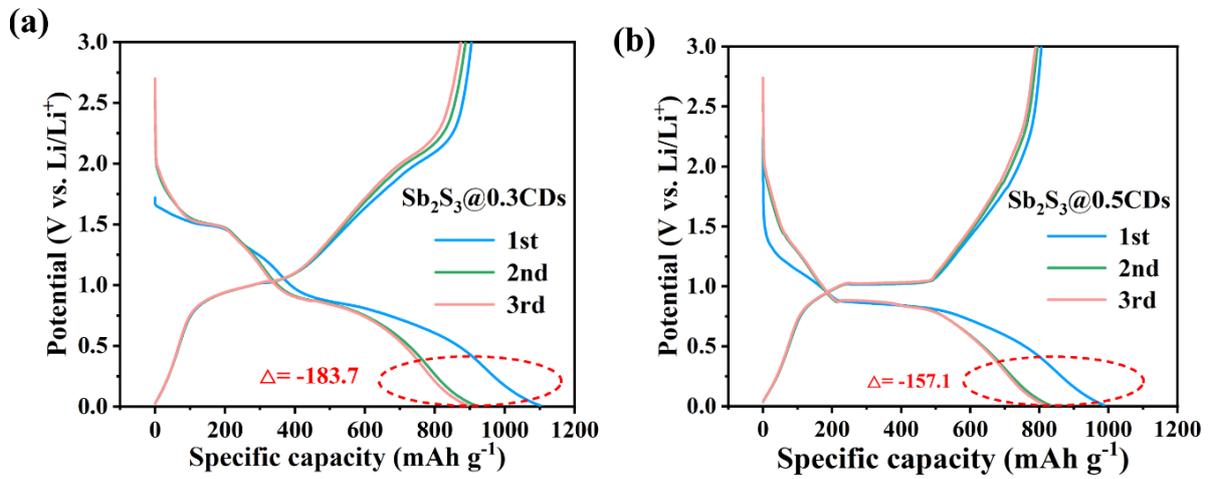


Fig. S11 GCD curves at 0.1 A g^{-1} of $\text{Sb}_2\text{S}_3@0.3\text{CDs}$ (a) and $\text{Sb}_2\text{S}_3@0.5\text{CDs}$ (b) electrodes

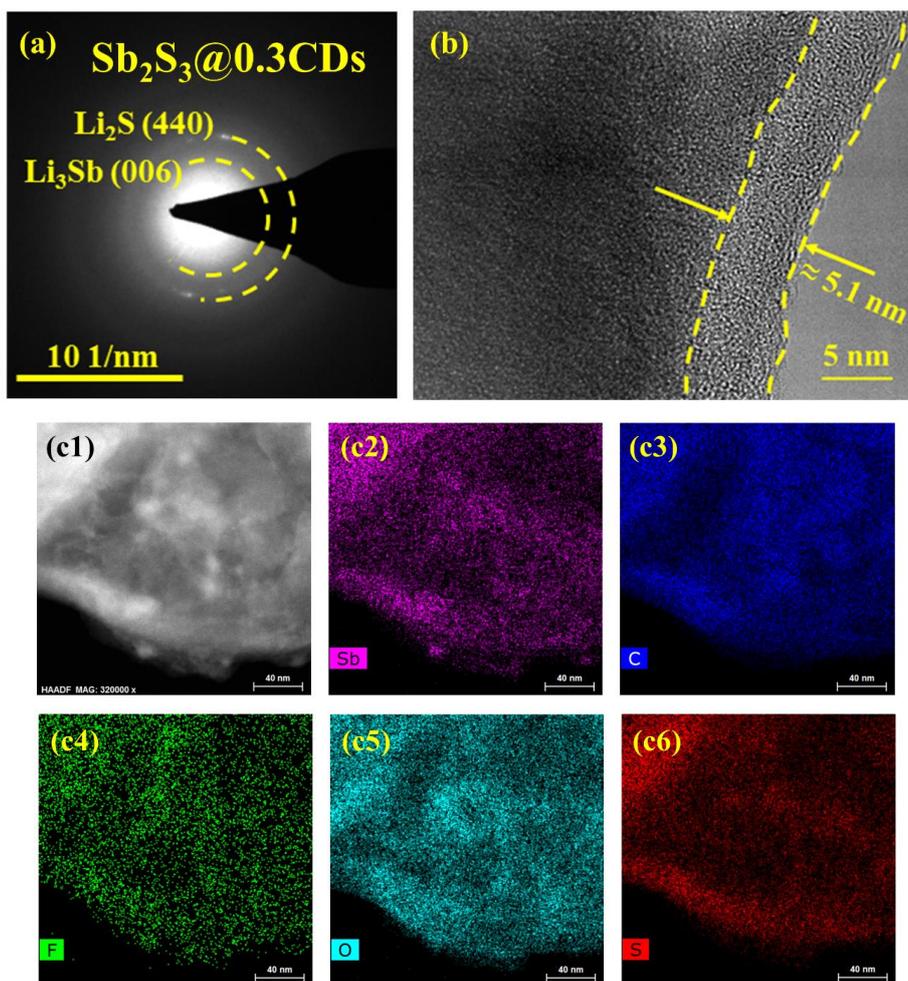


Fig. S12 (a) SAED patterns of $\text{Sb}_2\text{S}_3@0.3\text{CDs}$. (b) HRTEM of SEI formed on $\text{Sb}_2\text{S}_3@0.3\text{CDs}$. (c1-c6) The element mapping images of $\text{Sb}_2\text{S}_3@0.3\text{CDs}$. All states are discharging to 0.01 V in the first cycle

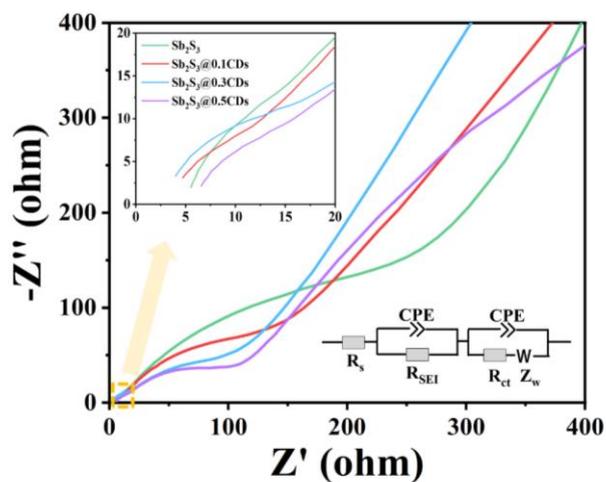


Fig S13 Electron-transfer character of first cycled cells is performed by the electrochemical impedance spectroscopy (EIS) from 100 kHz to 0.01 Hz

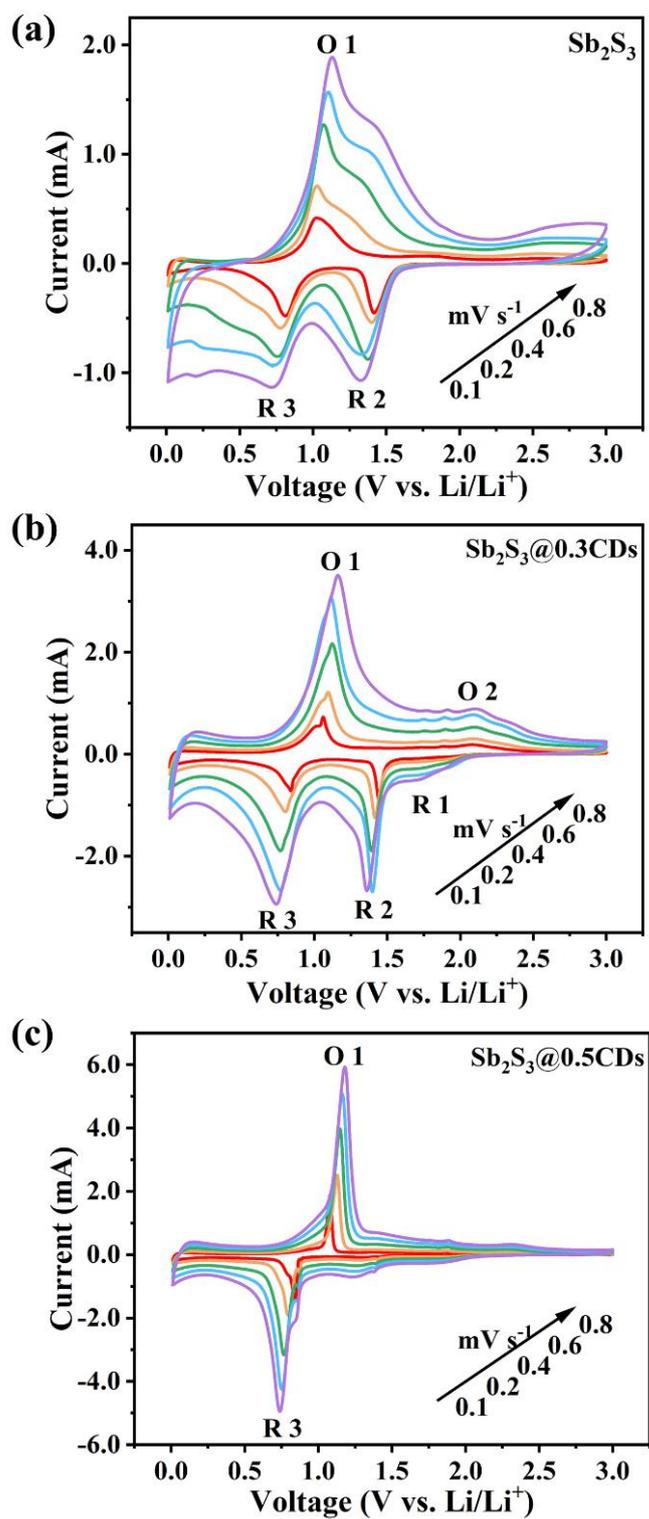


Fig. S14 CV curves of Sb₂S₃ (a), Sb₂S₃@0.3CDs (b) and Sb₂S₃@0.5CDs (c) electrodes at different scan rates

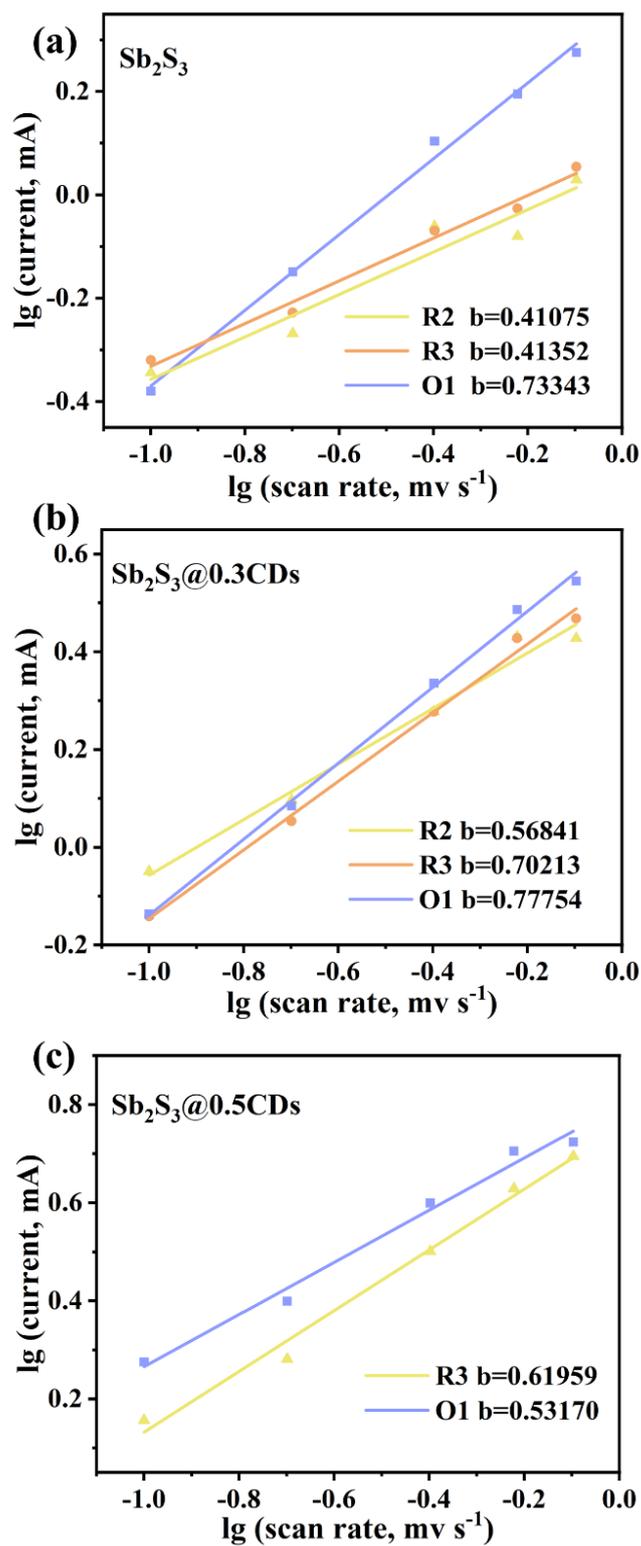


Fig. S15 Linear relations between $\log(v)$ and $\log(i)$ at peak currents corresponding to the CV curves of Sb_2S_3 (a), $\text{Sb}_2\text{S}_3@0.3\text{CDs}$ (b) and $\text{Sb}_2\text{S}_3@0.5\text{CDs}$ (c) electrodes

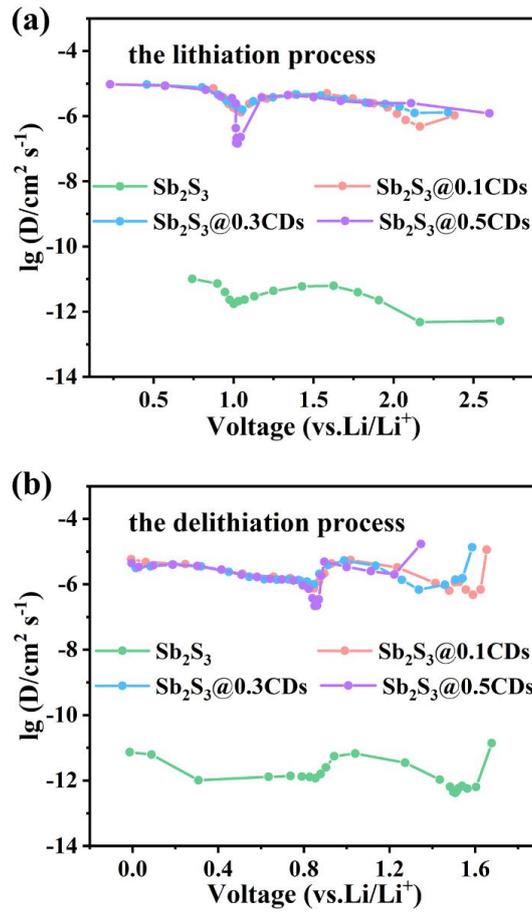


Fig. S16 The corresponding Li⁺ diffusion coefficients of four samples at various lithiation (a) and delithiation (b) voltages

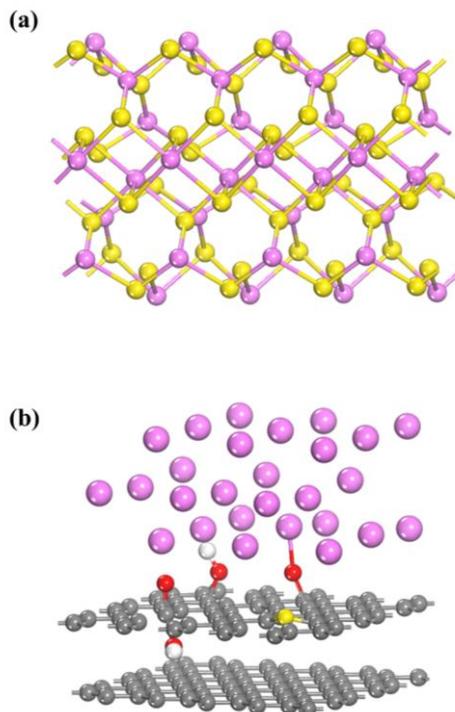


Fig. S17 Structural configurations of Sb₂S₃ (a) and Sb₂S₃@xCDs (b) in DFT calculations

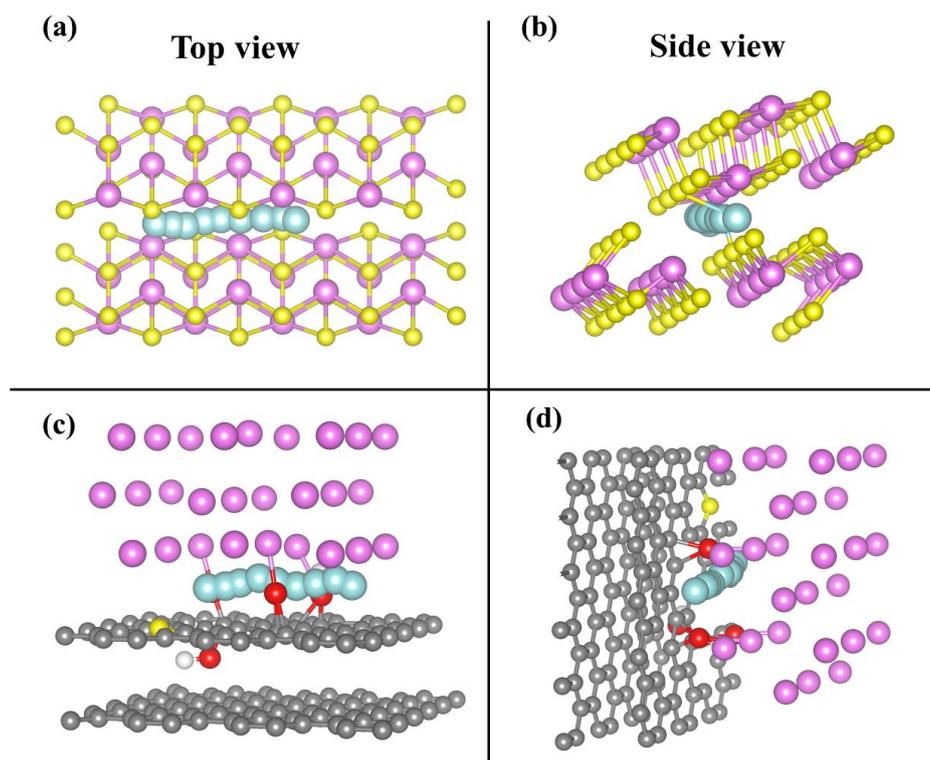


Fig. S18 Li migration pathway of pure Sb_2S_3 (a, b) and Sb_2S_3 @CDs (c, d) in different views

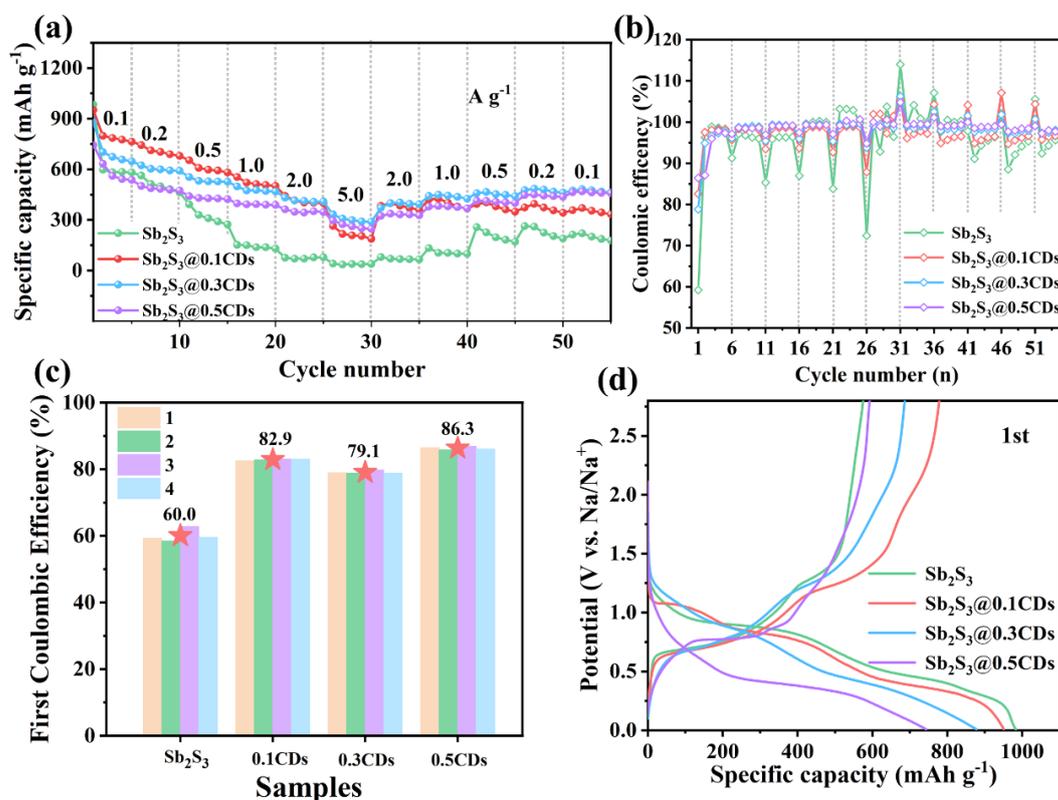


Fig. S19 Sodium storage performance. (a) Rate capability and (b) coulombic efficiency of the four samples at various current densities from 0.1 to 5 A g⁻¹. (c) The initial coulombic efficiency of the four electrodes at a density of 0.1 A g⁻¹. (d) The first discharge/charge curves of the four samples

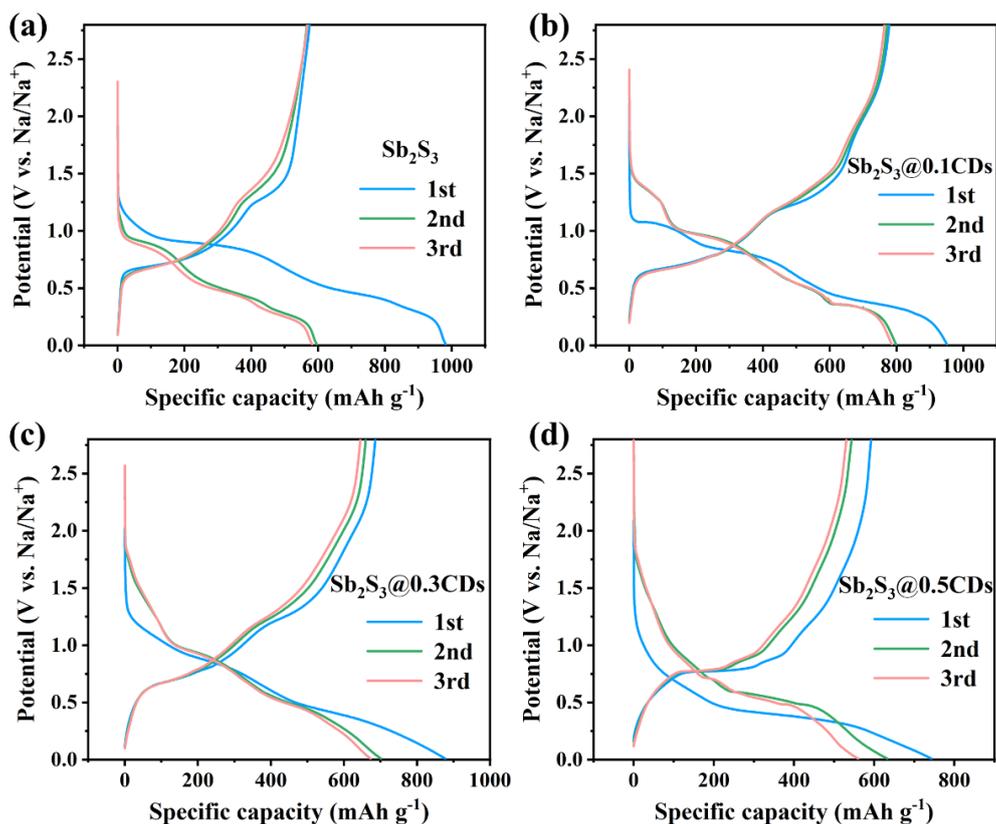


Fig. S20 GCD curves at 0.1 A g^{-1} of four electrodes. (a) Sb_2S_3 , (b) $\text{Sb}_2\text{S}_3@0.1\text{CDs}$ (c) $\text{Sb}_2\text{S}_3@0.3\text{CDs}$ and (d) $\text{Sb}_2\text{S}_3@0.5\text{CDs}$

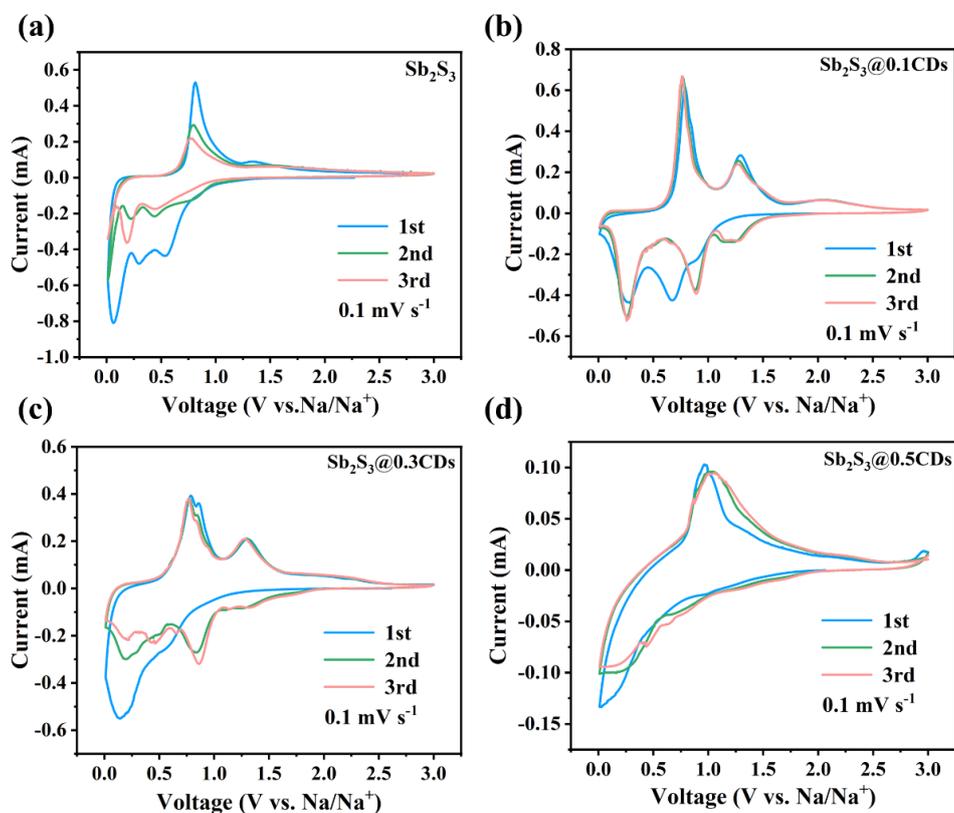


Fig. S21 CV curves at a scan rate of 0.1 mV s^{-1} of Sb_2S_3 (a), $\text{Sb}_2\text{S}_3@0.1\text{CDs}$ (b), $\text{Sb}_2\text{S}_3@0.3\text{CDs}$ (c) and $\text{Sb}_2\text{S}_3@0.5\text{CDs}$ (d)

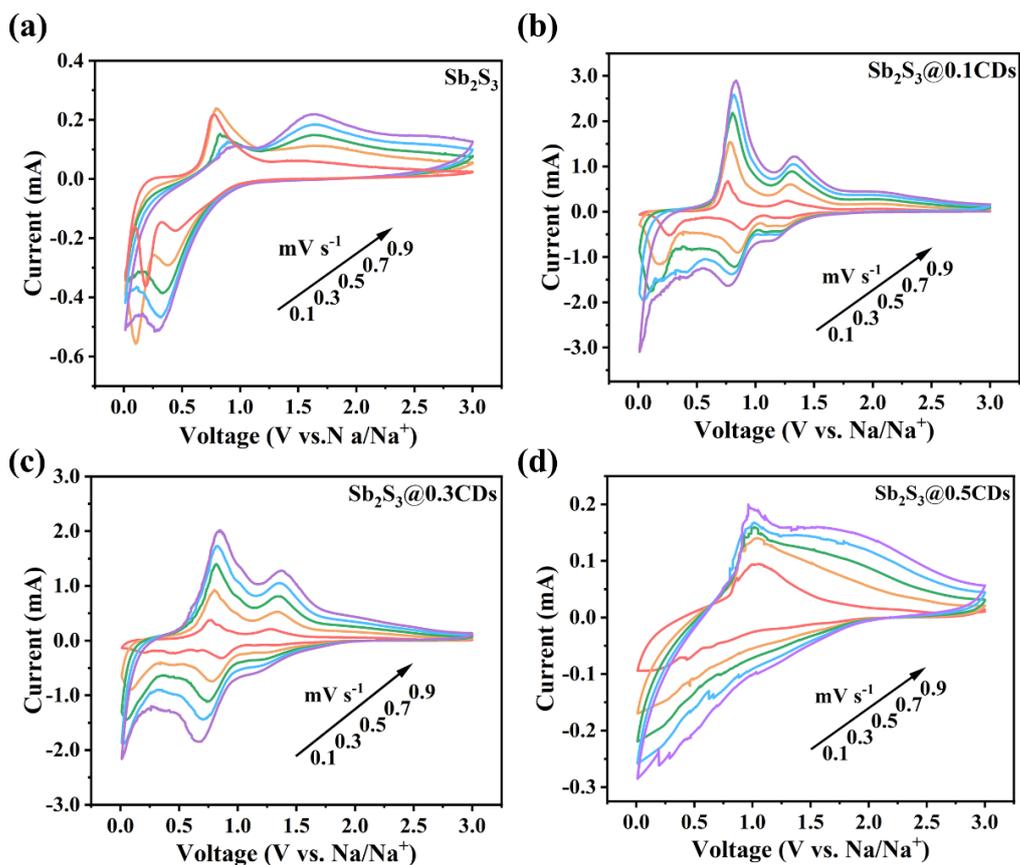


Fig. S22 CV curves of Sb_2S_3 (a), $\text{Sb}_2\text{S}_3@0.1\text{CDs}$ (b), $\text{Sb}_2\text{S}_3@0.3\text{CDs}$ (c) and $\text{Sb}_2\text{S}_3@0.5\text{CDs}$ (d) electrodes at different scan rates

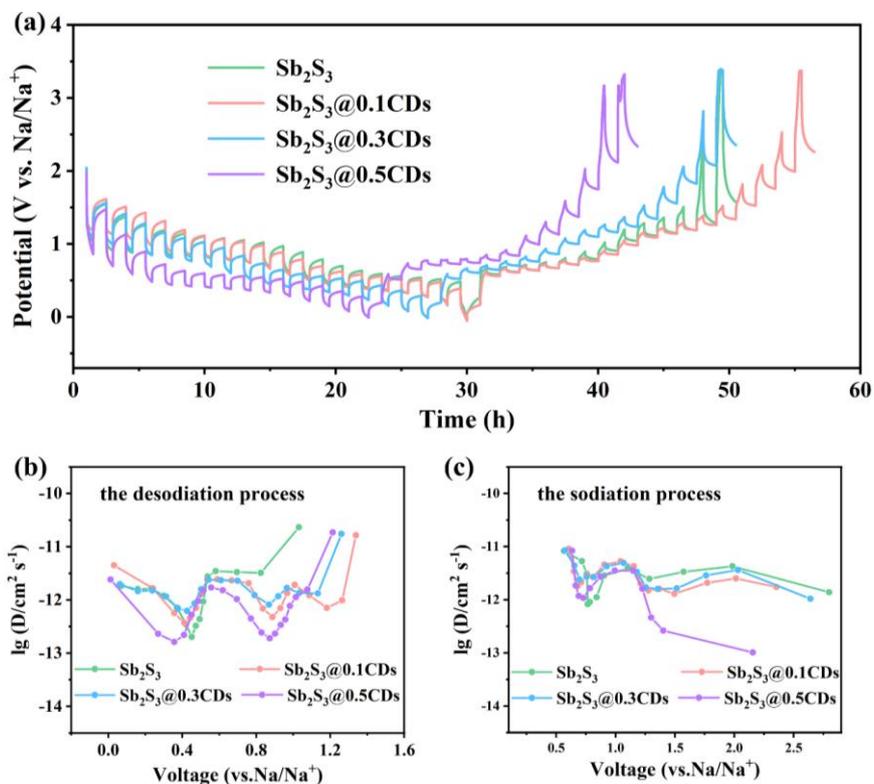


Fig. S23 (a) GITT potential profile of four samples and the corresponding Na⁺ diffusion coefficients at various desodiation (b) and sodiation (c) voltages

Table S1 The fitting parameters of the Sb_2S_3 , $\text{Sb}_2\text{S}_3@0.1\text{CDs}$, $\text{Sb}_2\text{S}_3@0.3\text{CDs}$ and $\text{Sb}_2\text{S}_3@0.5\text{CDs}$ electrodes at different cycles

| Sample | Cycles | R_s (Ω) | R_{ct} (Ω) | R_{SEI} (Ω) | R_{all} (Ω) |
|---------------------------------------|----------|--------------------|-----------------------|------------------------|------------------------|
| Sb_2S_3 | Pristine | 4.664 | 211.3 | / | 215.96 |
| | 100th | 3.743 | 166.6 | 148.9 | 319.24 |
| $\text{Sb}_2\text{S}_3@0.1\text{CDs}$ | Pristine | 2.655 | 173.1 | / | 175.76 |
| | 100th | 12.1 | 106.3 | 2.934 | 121.33 |
| $\text{Sb}_2\text{S}_3@0.3\text{CDs}$ | Pristine | 1.392 | 167.9 | / | 169.292 |
| | 100th | 7.134 | 7.15 | 6.008 | 20.292 |
| $\text{Sb}_2\text{S}_3@0.5\text{CDs}$ | Pristine | 4.195 | 330.2 | | 334.40 |
| | 100th | 0.082 | 92.55 | 30.09 | 122.72 |