

Interfaces engineering in NiSe₂/Ni₂Co/CoSe₂ heterostructures encapsulated in hollow carbon shell for high-rate Li-Se batteries

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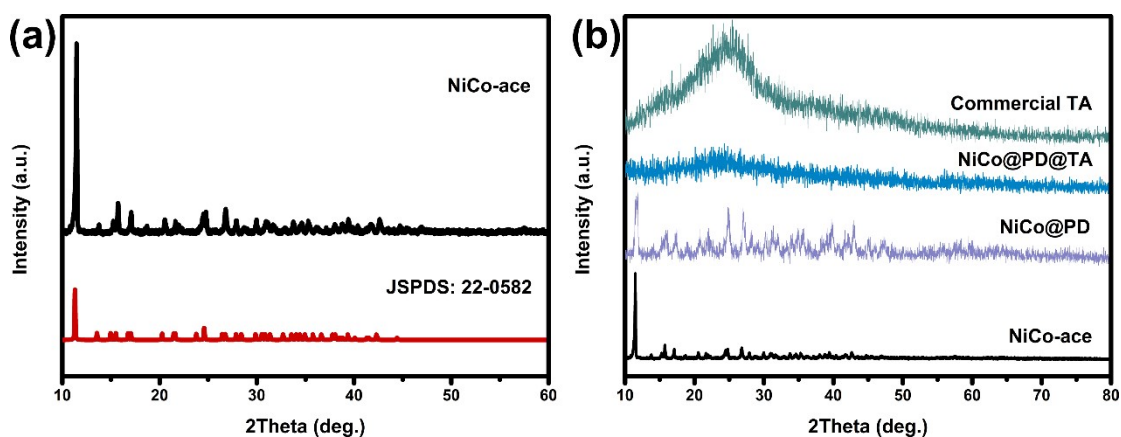


Fig. S1 XRD patterns of (a) precursor NiCo-ace and (b) intermediate products NiCo-ace@PD and NiCo@PD@TA.

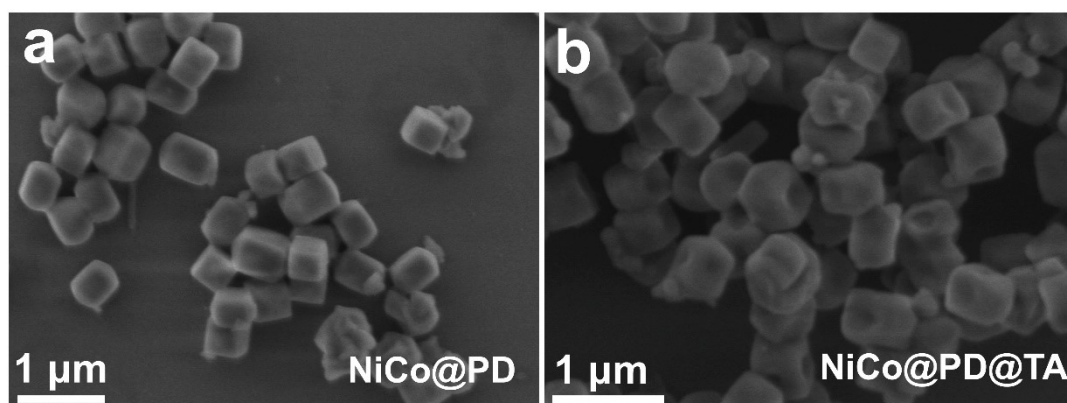


Fig. S2 SEM images of intermediates (a) NiCo@PD and NiCo@PD@TA.

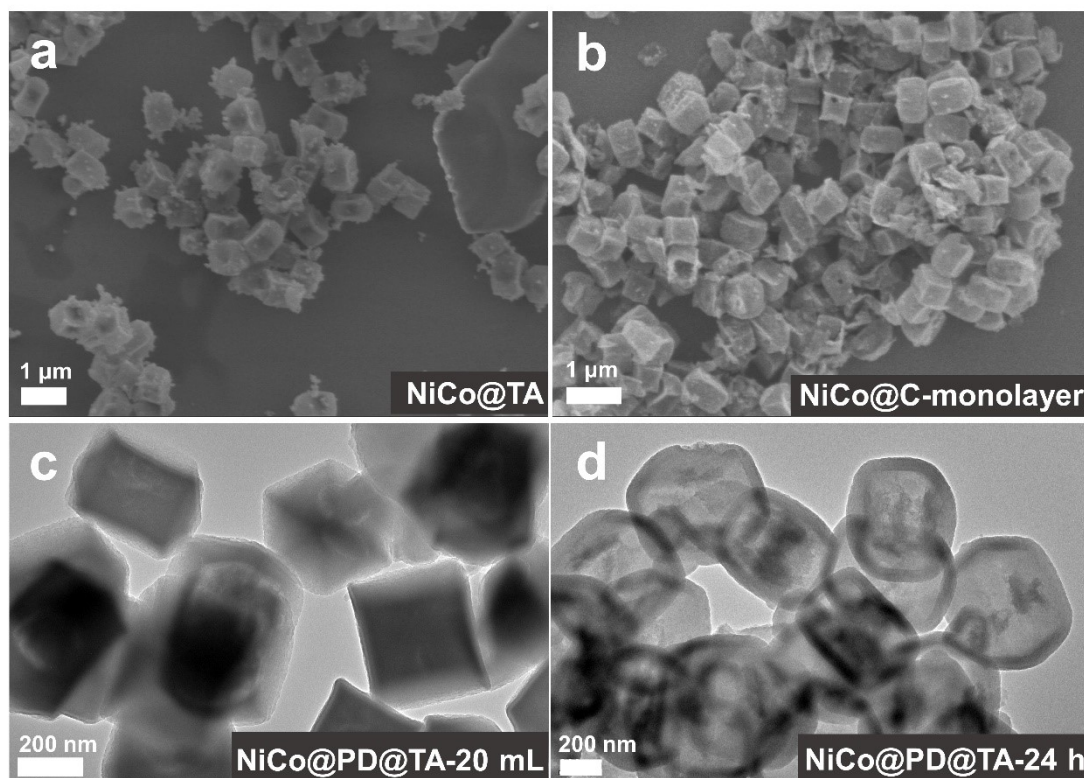


Fig. S3 SEM images of contrast samples (a) NiCo@TA without PD layer and (b) corresponding carbonized product NiCo@C-monolayer, (c) NiCo@PD@TA-20 mL, (d) NiCo@PD@TA-24 h.

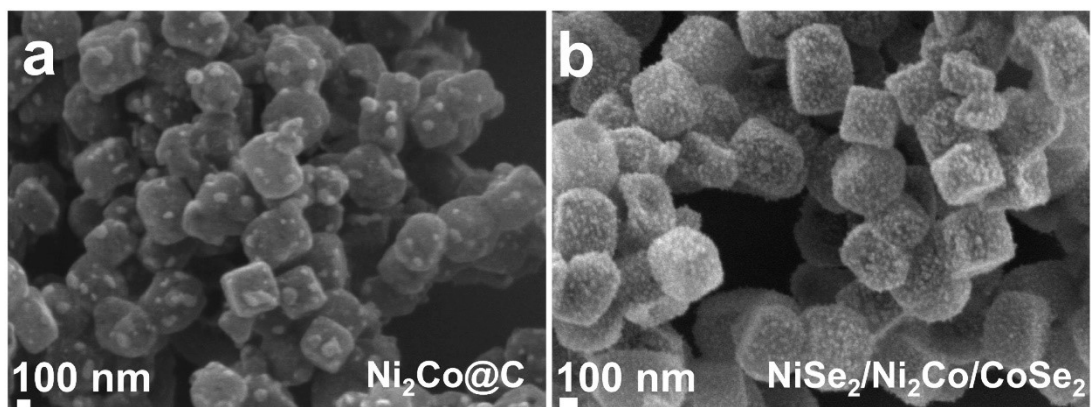


Fig. S4 SEM images of (a) $\text{Ni}_2\text{Co}@C$ and (b) $\text{NiSe}_2/\text{Ni}_2\text{Co}/\text{CoSe}_2$.

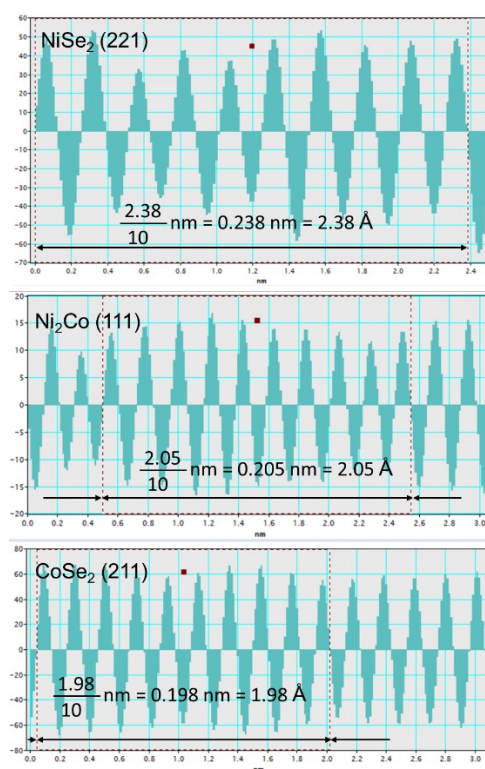


Fig. S5 The profiles of corresponding intensity variations to determine crystal plane spacing in Figure 2c.

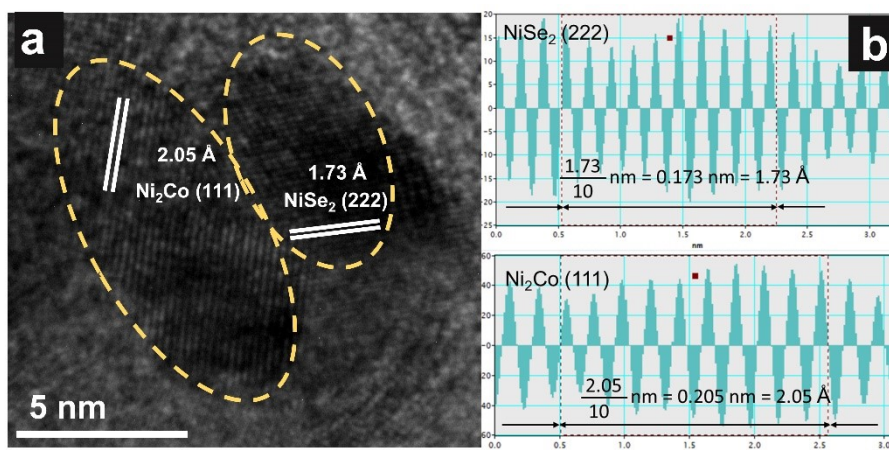


Fig. S6 (a) The heterointerface of Ni_2Co and NiSe_2 and (b) the profiles of corresponding intensity variations of crystal plane spacing.

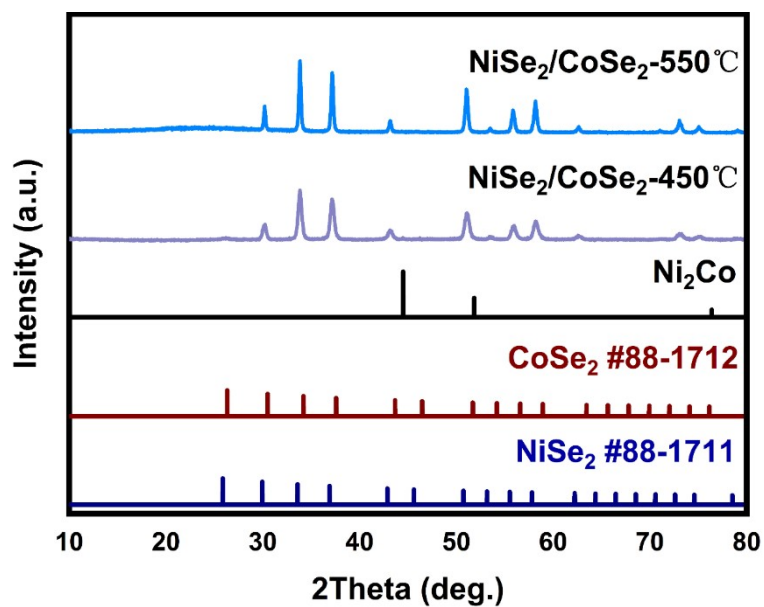


Fig. S7 XRD patterns of contrast samples heterogeneous $\text{NiSe}_2/\text{CoSe}_2$.

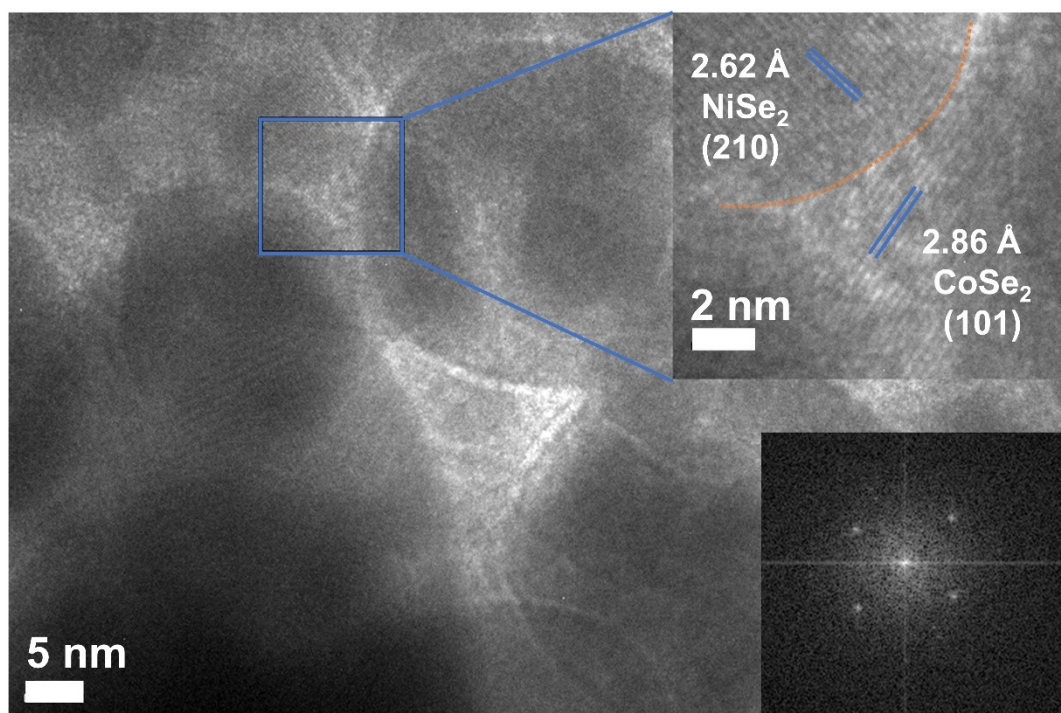


Fig. S8 The HRTEM image of contrast sample $\text{NiSe}_2/\text{CoSe}_2$ with single heterointerface.

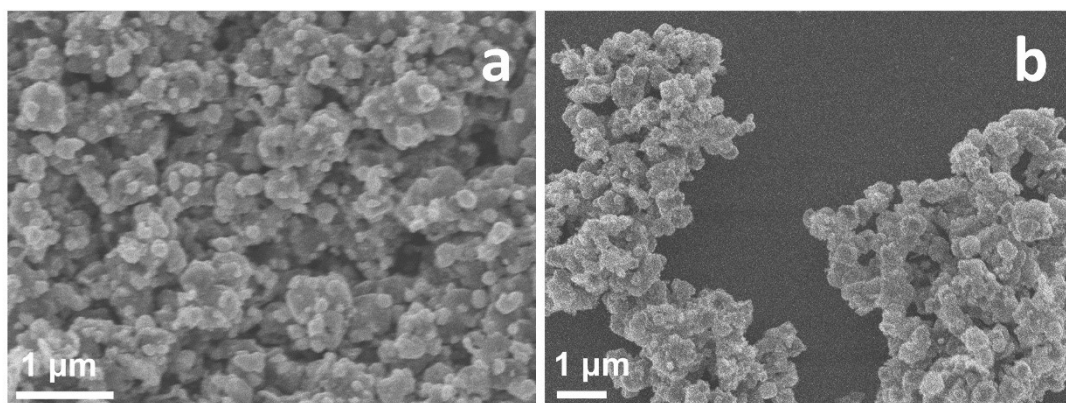


Fig. S9 SEM images of (a) $\text{NiSe}_2/\text{CoSe}_2@\text{Se}$ and (b) $\text{NiSe}_2/\text{Ni}_2\text{Co}/\text{CoSe}_2@\text{Se}$.

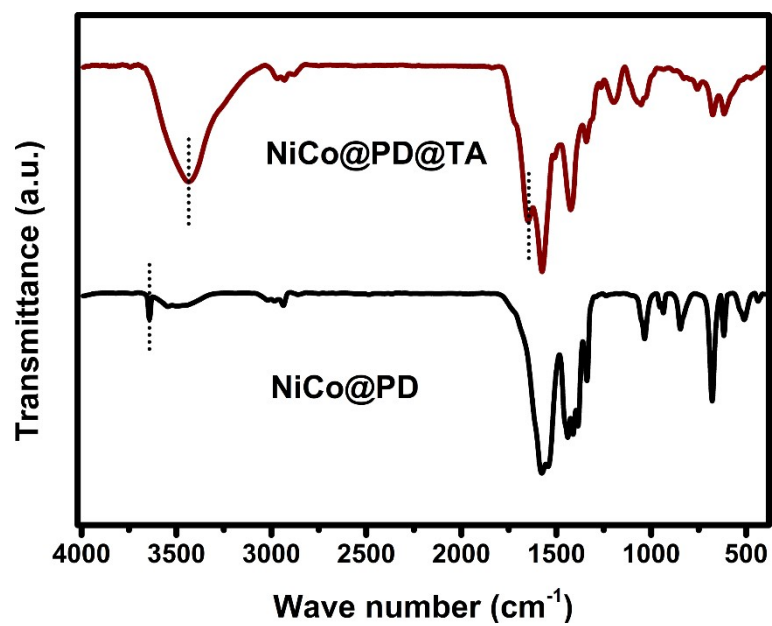


Fig. S10 The FTIR spectra of intermediate products NiCo@PD and NiCo@PD@TA.

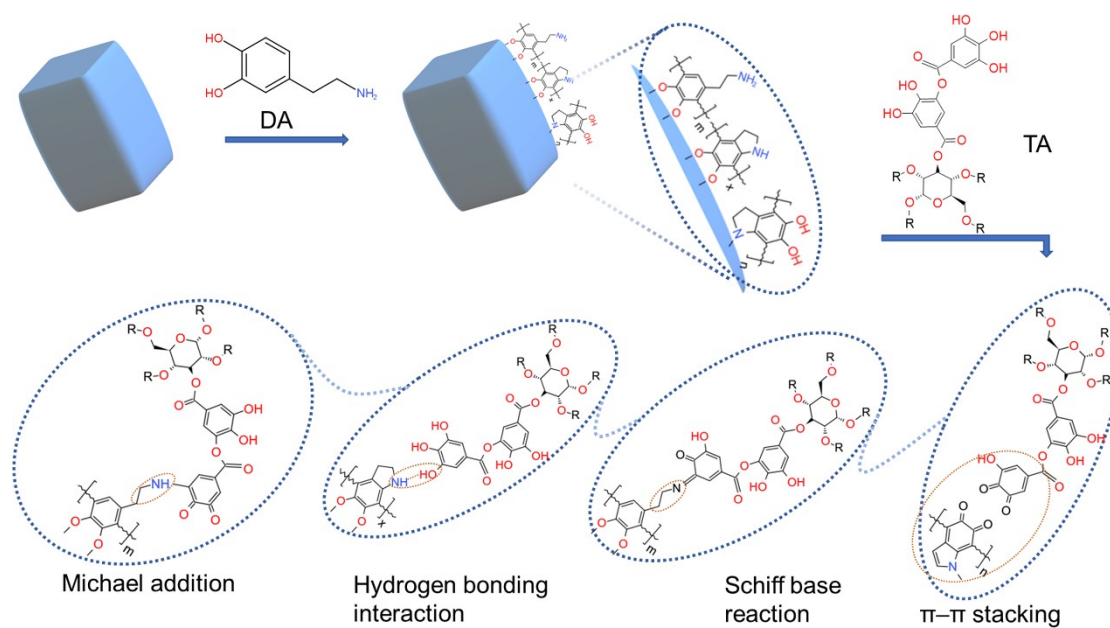


Fig. S11 The schematic illustration of the linking process between PD layer and TA layer with four possible functional group reactions.

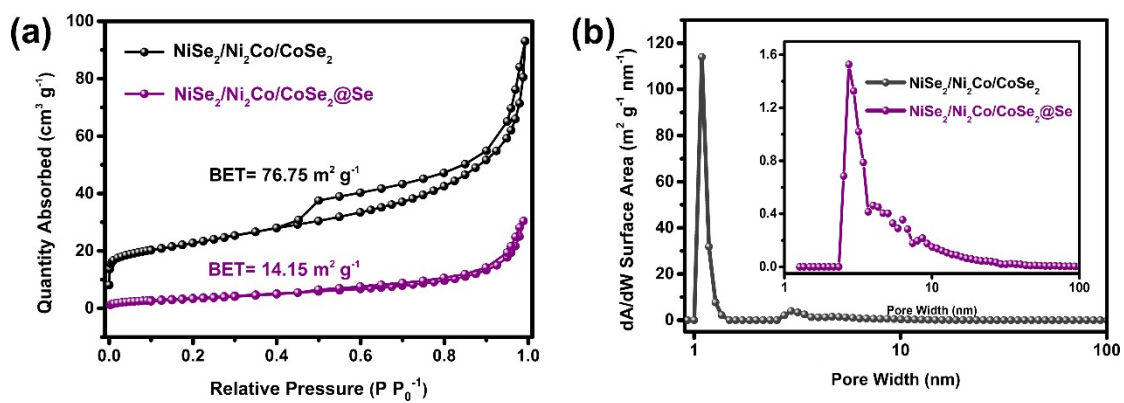


Fig. S12 (a) The nitrogen adsorption–desorption isotherms and (b) the pore size distribution of $\text{NiSe}_2/\text{Ni}_2\text{Co}/\text{CoSe}_2$ and $\text{NiSe}_2/\text{Ni}_2\text{Co}/\text{CoSe}_2@\text{Se}$.

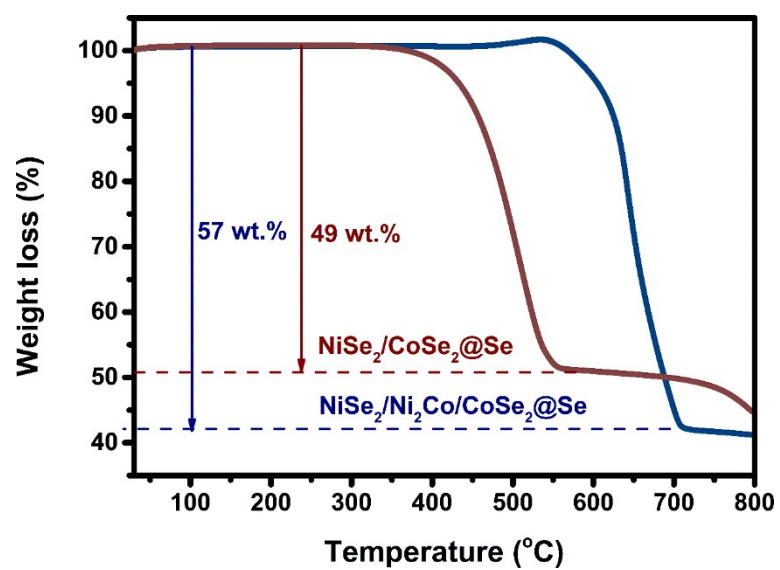


Fig. S13 The TG curves of $\text{NiSe}_2/\text{Ni}_2\text{Co}/\text{CoSe}_2@\text{Se}$ and $\text{NiSe}_2/\text{CoSe}_2@\text{Se}$ in N_2 atmosphere.

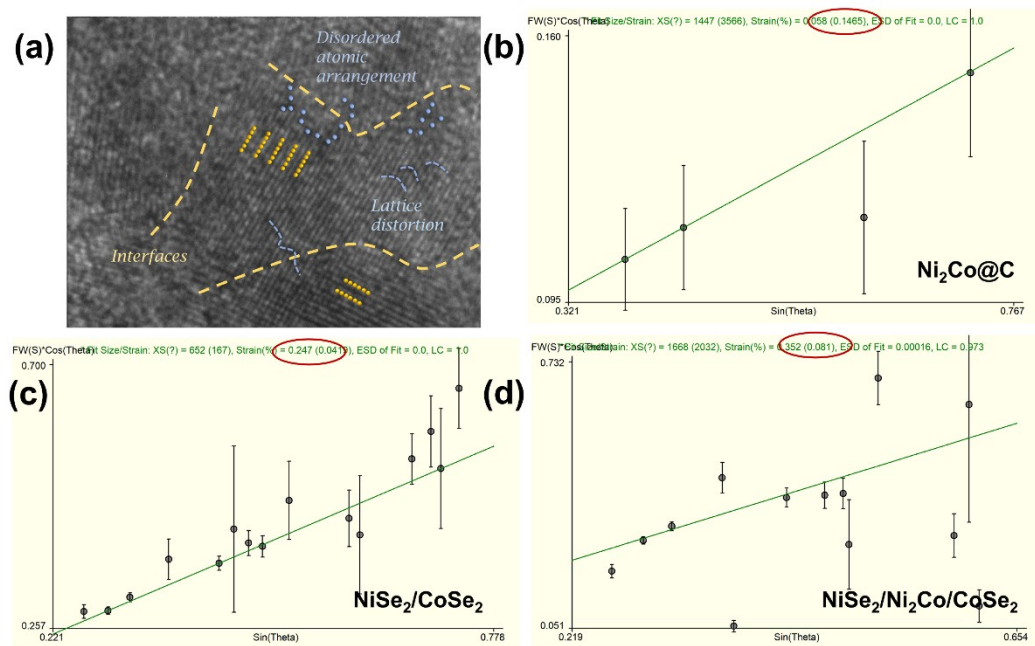


Fig. S14 (a) The scheme of subtle distortion at heterointerfaces. (b-c) Size and strain plots of $\text{Ni}_2\text{Co}@C$, $\text{NiSe}_2/\text{CoSe}_2$ and $\text{NiSe}_2/\text{Ni}_2\text{Co}/\text{CoSe}_2$ calculated by XRD Patterns in software MDI Jade 6.

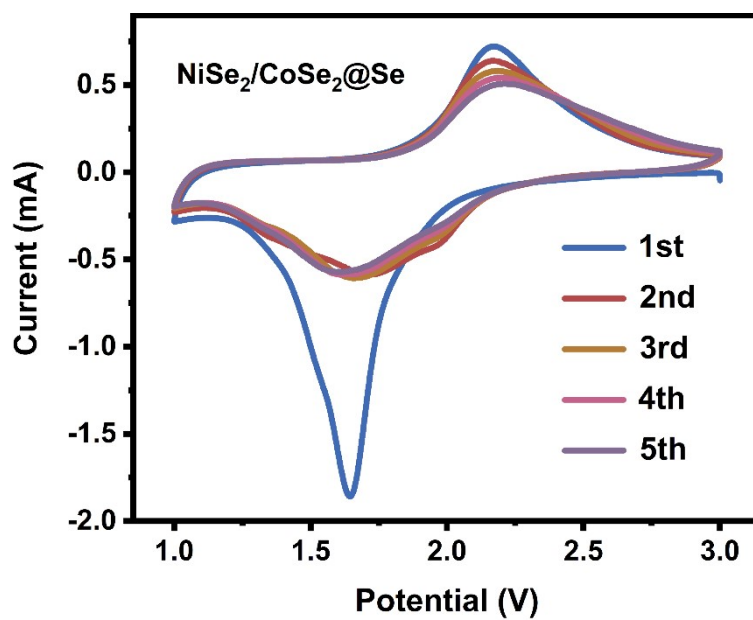


Fig. S15 CV curves of $\text{NiSe}_2/\text{CoSe}_2@\text{Se}$ cathode at 0.2 mV s^{-1} in Li-Se batteries.

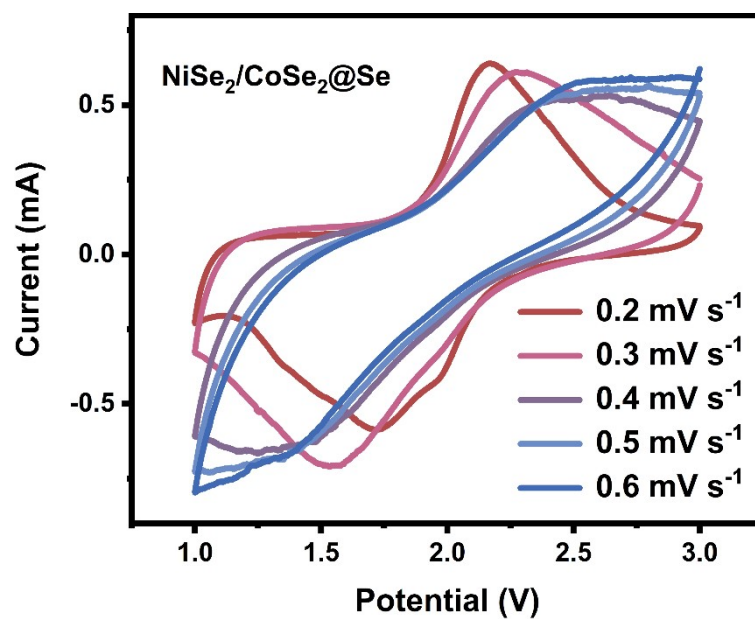


Fig. S16 CV curves of $\text{NiSe}_2/\text{CoSe}_2@\text{Se}$ cathode from 0.2 to 0.6 mV s^{-1} in Li-Se batteries.

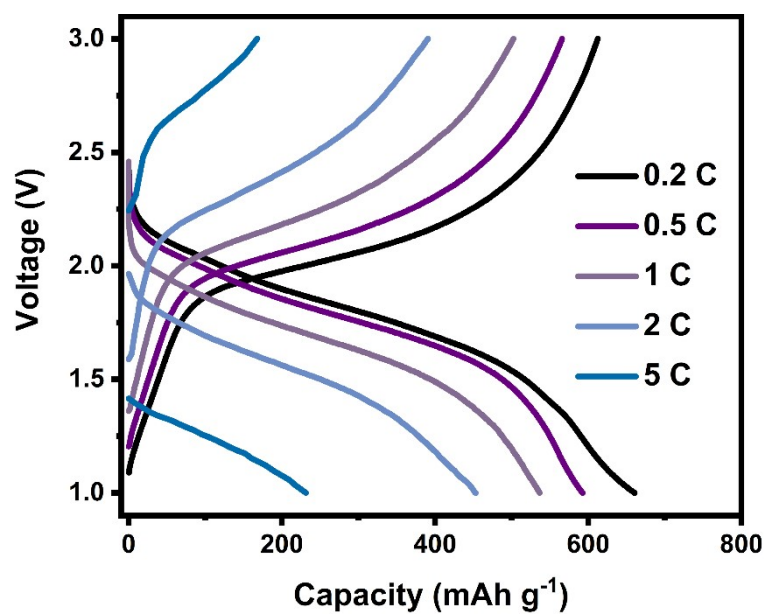


Fig. S17 The galvanostatic charge-discharge curves at 0.2 C of $\text{NiSe}_2/\text{Ni}_2\text{Co}/\text{CoSe}_2@\text{Se}$.

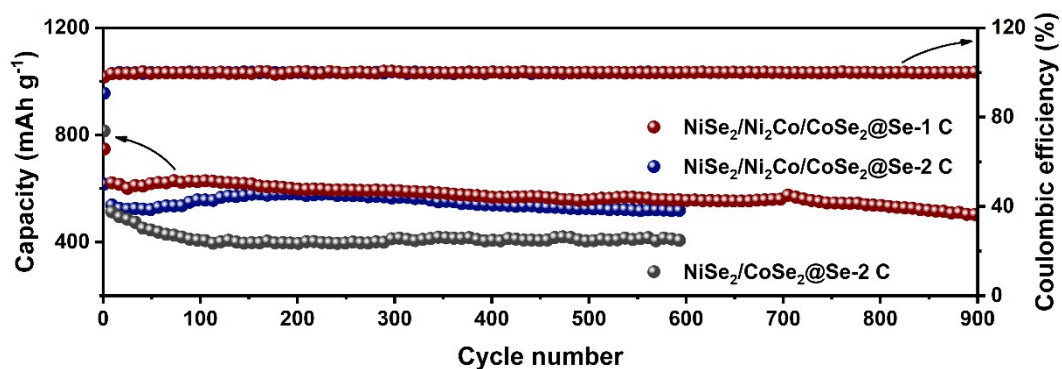


Fig. S18 Cycling performance of $\text{NiSe}_2/\text{Ni}_2\text{Co}/\text{CoSe}_2@\text{Se}$ and $\text{NiSe}_2/\text{CoSe}_2@\text{Se}$ (Se loading: 0.9 mg cm^{-2}).

Table S1. Comparison of electrochemical performances of $\text{NiSe}_2/\text{Ni}_2\text{Co}/\text{CoSe}_2@\text{Se}$ with other carbonaceous hosts for Li-Se batteries reported in literatures.

Material	Current density ($1\text{C}=675\text{mA g}^{-1}$)	Cycle number	Capacity (mAh g^{-1})
$\text{Se}@\text{CoSe}_2\text{-PC}^1$	1 C	100	408
$\text{Se}@\text{Co}_{\text{SA}}\text{-HC}^2$	5 C	1500	340
$\text{PANI}@\text{Se/C-G}^3$	2 C	500	528.6
A4-carbon/ Se^4	3 C	2000	343
HPC/ Se^5	2 C	800	451
NS-K-PC/ Se^6	1 C	500	394.2
$\text{Se}@\text{HHCS}^7$	10 C	2000	357
Se/CZIF-5^8	1 C	700	400
This work	1 C	900	503
	2 C	600	515
	12 C	2200	324

References

1. H. Tian, H. Tian, S. Wang, S. Chen, F. Zhang, L. Song, H. Liu, J. Liu and G. Wang, *Nature communications*, 2020, **11**, 1-12.
2. X. Wang, Y. Tan, Z. Liu, Y. Fan, M. Li, H. A. Younus, J. Duan, H. Deng and S. Zhang, *Small*, 2020, **16**, 2000266.
3. J. Yang, H. Gao, D. Ma, J. Zou, Z. Lin, X. Kang and S. Chen, *Electrochimica Acta*, 2018, **264**, 341-349.
4. G. D. Park, J. H. Kim, J.-K. Lee and Y. C. Kang, *Journal of Materials Chemistry A*, 2018, **6**, 21410-21418.
5. L. Cheng, C. Ma, W. Lu, X. Wang, H. Yue, D. Zhang and Z. Xing, *Chemical Engineering Journal*, 2022, **433**, 133527.
6. Q. Xia, J. Hu, Q. Chen and L. Zhang, *J. Colloid Interface Sci.*, 2022, **610**, 643-652.
7. Y. Wang, H. Hao, S. Hwang, P. Liu, Y. Xu, J. A. Boscoboinik, D. Datta and D. Mitlin, *Journal of Materials Chemistry A*, 2021, **9**, 18582-18593.
8. M. H. Aboonasr Shiraz, E. Rehl, H. Kazemian and J. Liu, *Nanomaterials*, 2021, **11**, 1976.