Supplementary Information (SI) for Journal of Materials Chemistry A. This journal is © The Royal Society of Chemistry 2024

Supporting Information for

Enhanced Electrochemical Performance of NiSbS/NiSb/NiS Nanocomposites

Anchored on Graphite Nanosheets for Sodium-Ion Battery Applications

Shandong Huang^a, Dong Feng^{b, c*}, Yuanzhi Zhu^b, Yihong Ding^{a*}, Delong Xie^{b, c}, Yi Mei^{b, c}, Tianbiao Zeng^{a*} a. Key Laboratory of Carbon Materials of Zhejiang Province, Wenzhou Key Lab of Advanced Energy Storage and Conversion, Zhejiang Province Key Lab of Leather Engineering, College of Chemistry and Materials Engineering, Wenzhou University, Wenzhou, Zhejiang 325035, China

b. Yunnan Provincial Key Laboratory of Energy Saving in Phosphorus Chemical Engineering and New Phosphorus Materials, Faculty of Chemical Engineering, Kunming University of Science and Technology, Kunming 650500, China

c. The International Joint Laboratory for Sustainable Polymers of Yunnan Province, Kunming 650500, China

*: Corresponding author: <u>fdryan@kust.edu.cn</u> (D. Feng), <u>yhdd@wzu.edu.cn</u> (Y. Ding) <u>tianbiaozeng@126.com</u> (T. Zeng)

Materials	Ni	Sb_2S_3	NiSbS	NiSb
Crystal ID	mp-23	mp-2809	mp-3679	mp-810
Energy eV/atom	-5.7798	-4.3828	-4.9969	-5.2253
Materials	NiS	NiS ₂	Ni ₃ S ₄	Ni ₃ S ₂
Crystal ID	mp-1547	mp-1180046	mp-1050	mp-362
Energy eV/atom	-5.3168	-4.9412	-5.2125	-5.4933
Materials	NiSb ₂	Sb	Ni ₃ Sb	Ni ₅ Sb ₂
Crystal ID	mp-19895	mp-104	mp-672371	mp-2409
Energy eV/atom	-4.8767	-4.129	-5.5154	-5.4786
Materials	Na ₂ S	Na ₃ Sb	Na	S
Crystal ID	mp-648	mp-7956	mp-10172	mp-96
Energy eV/atom	-3.3241	-2.4524	-1.3122	-4.1364

 Table S1 The final energy/atom of some reactants.

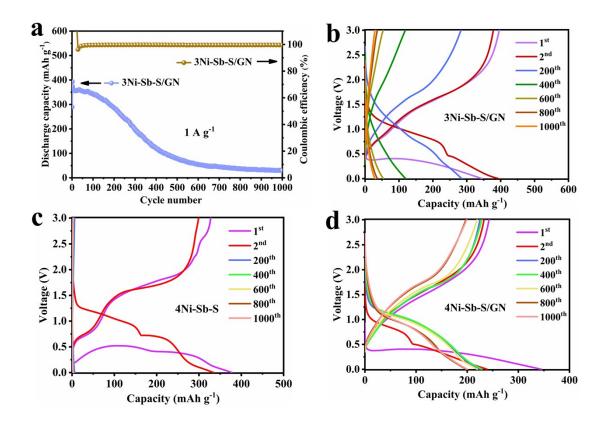


Fig. S1. (a) Cycling stability of 3Ni-Sb-S/GN at a current density of 1.0 A g⁻¹; Discharge/charge profiles of (b) 3Ni-Sb-S/GN, (c) 4Ni-Sb-S and (d) 4Ni-Sb-S/GN at a current density of 1.0 A g⁻¹.

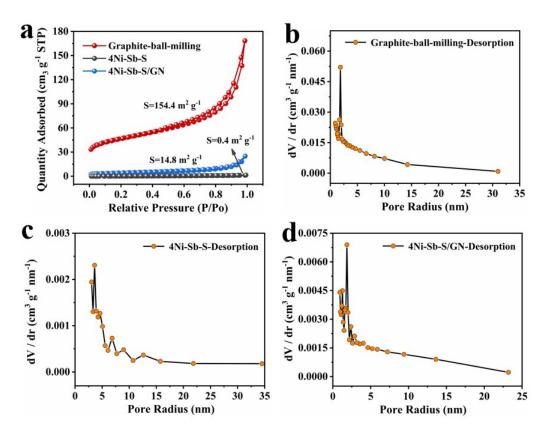


Fig. S2. Nitrogen adsorption isotherms of Graphite-ball-milling, 4Ni-Sb-S, and 4Ni-Sb-S/GN (a); Corresponding pore size distribution of (b) Graphite-ball-milling, (c) 4Ni-Sb-S, and (d) 4Ni-Sb-S/GN.

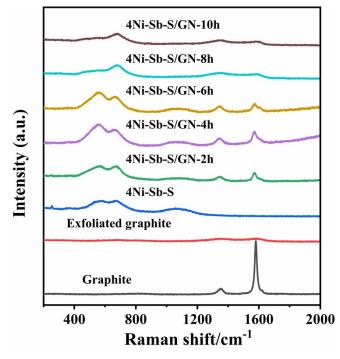


Fig. S3. Raman patterns of Graphite, Exfoliated graphite, 4Ni-Sb-S, and 4Ni-Sb-S/GN at different milling times.

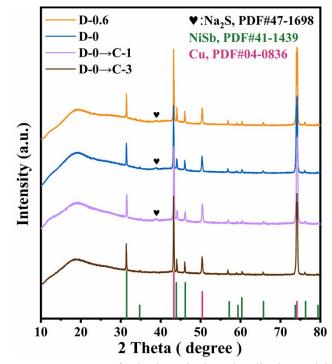


Fig. S4. *Ex*-situ XRD patterns of Ni-Sb-S during the discharge/charge processes.

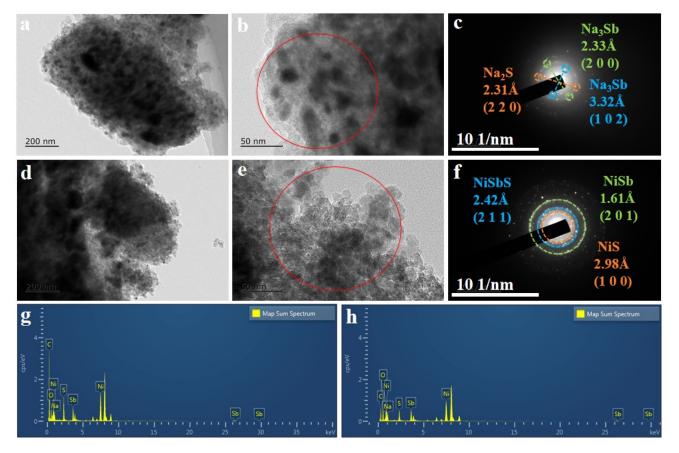


Fig. S5. (a, b) Supplemented TEM image of Ni-Sb-S/GN electrode after discharging to 0V; (c) SAED images of Ni-Sb-S/GN in image (b); (d, e) supplemented TEM images of Ni-Sb-S/GN after discharging to 0V followed by charging to 3V; (f) SAED images of Ni-Sb-S/GN in image (e). (g) The elementary distributions of image (b); (h) The elementary distributions of image (e).

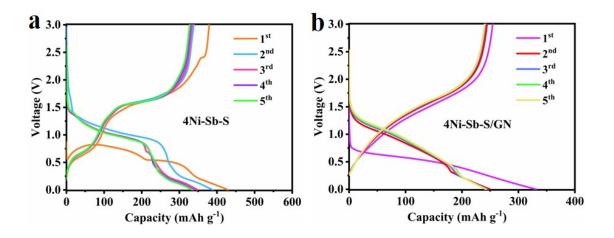


Fig. S6. Discharge/charge profiles of (a) 4Ni-Sb-S and (b) 4Ni-Sb-S/GN.

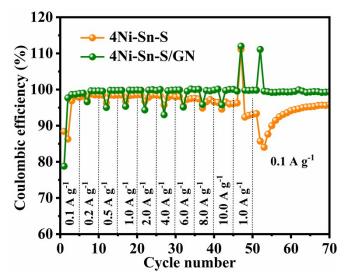


Fig. S7. Coulombic efficiency of 4Ni-Sb-S and 4Ni-Sb-SGN tested from 0.1~10.0 A g⁻¹.

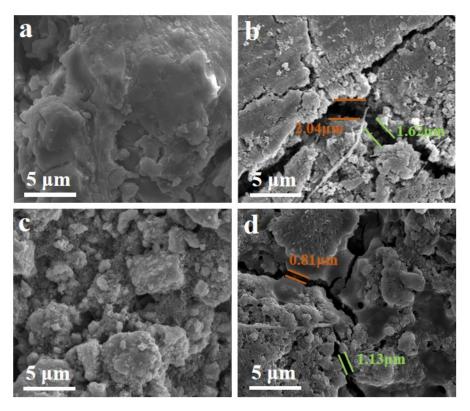


Fig. S8. SEM images of (a, b) Ni-Sb-S, and (c,d) Ni-Sb-S/GN before and after 1000 cycles at 1.0 A g⁻¹.

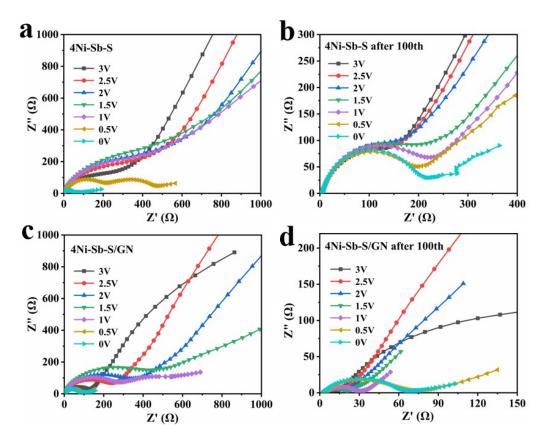


Fig. S9. Nyquist plots of the bare 4Ni-Sb-S, and 4Ni-Sb-S/GN electrodes before(a, c) and after cycling 100 cycles(b, d).

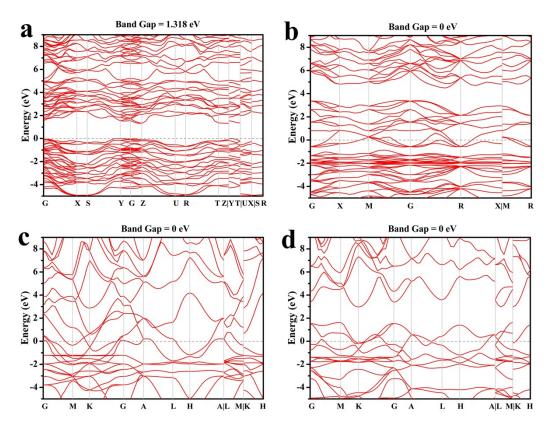


Fig. S10. Band gap values of (a) Sb₂S₃, (b) NiSbS, (c) NiSb, and (d) NiS.

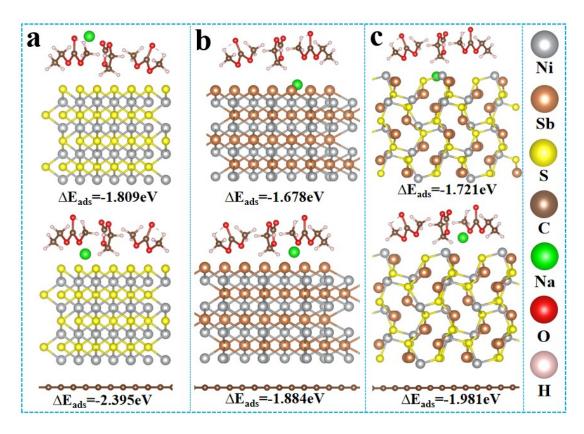


Fig. S11. Adsorption models and energies of adding (EC:DMC:EMC) (a) NiS, NiS/GN, (b) NiSb, NiSb/GN, and (c) NiSbS, NiSbS/GN.

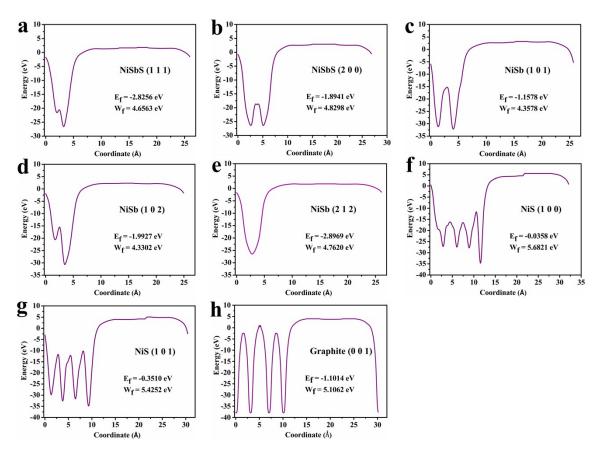


Fig. S12. The work functions of Graphite, NiSbS, NiSb, and NiS based on the observed lattice planes (*i.e.*, $(0\ 0\ 1)$ of Graphite; $(1\ 1\ 1)$ and $(2\ 0\ 0)$ of NiSbS; $(1\ 0\ 1)$, $(1\ 0\ 2)$, and $(2\ 1\ 2)$ of NiSb; $(1\ 0\ 0)$ and $(1\ 0\ 1)$ of NiS.

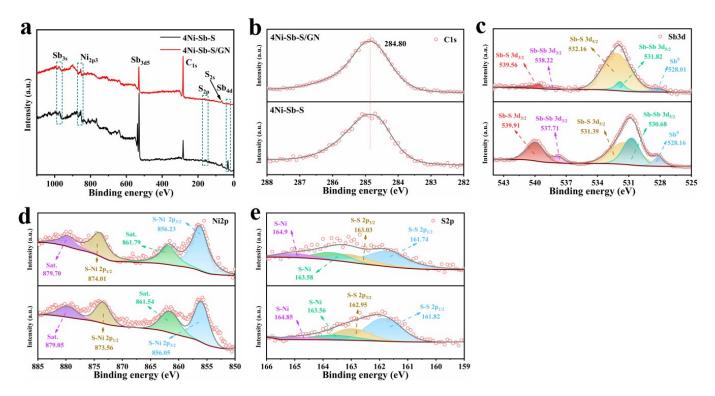


Fig. S13. The XPS spectra of 4Ni-Sb-S and 4Ni-Sb-S/GN. (a) survey spectra, (b) C 1s spectra, (c) Sb 3d spectra, (d) Ni 2p spectra, and (e) S 2p spectra.

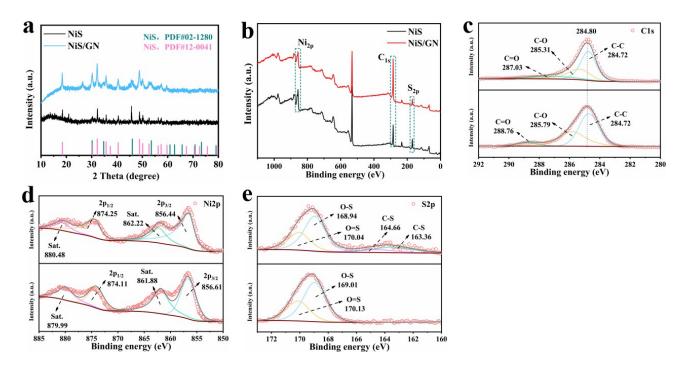


Fig. S14. (a) XRD patterns, and XPS spectra of NiS and NiS/GN. (b) survey spectra, (c) C 1s spectra, (d) Ni 2p spectra, and (e) S 2p spectra.

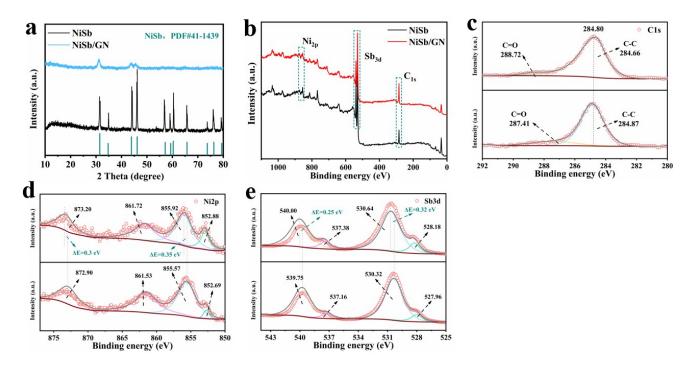


Fig. S15. (a) XRD patterns, and XPS spectra of NiSb and NiSb/GN. (b) survey spectra, (c) C 1s spectra, (d) Ni 2p spectra, and (e) Sb 3d spectra.

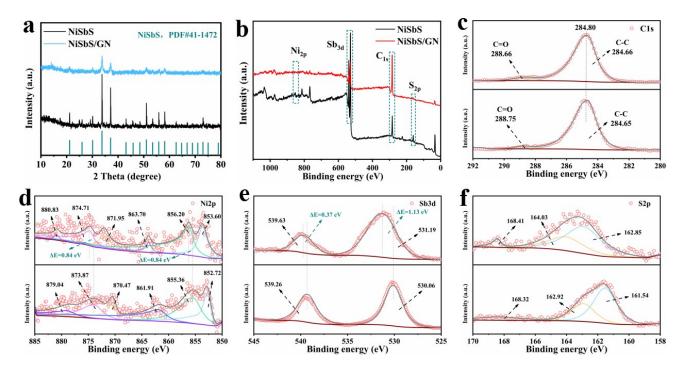


Fig. S16. (a) XRD patterns, and XPS spectra of NiSbS and NiSbS/GN. (b) survey spectra, (c) C 1s spectra, (d) Ni 2p spectra, (e) Sb 3d spectra, and (f) S 2p spectra.

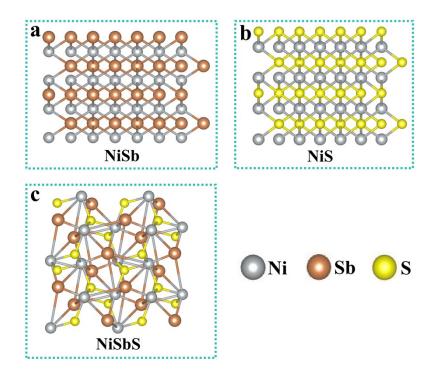


Fig. S17. The crystal stricture of (a) NiSb, (b) NiS, and (c) NiSbS.