Electronic Supplementary Information

$CuGaS_2$ nanoplates: a robust and self-healing anode for power battery in wide temperaturerange of 268-318 K

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Contents:

Table S1-S2

Experimental details Fig. S1-Fig. S5

References (1-8)

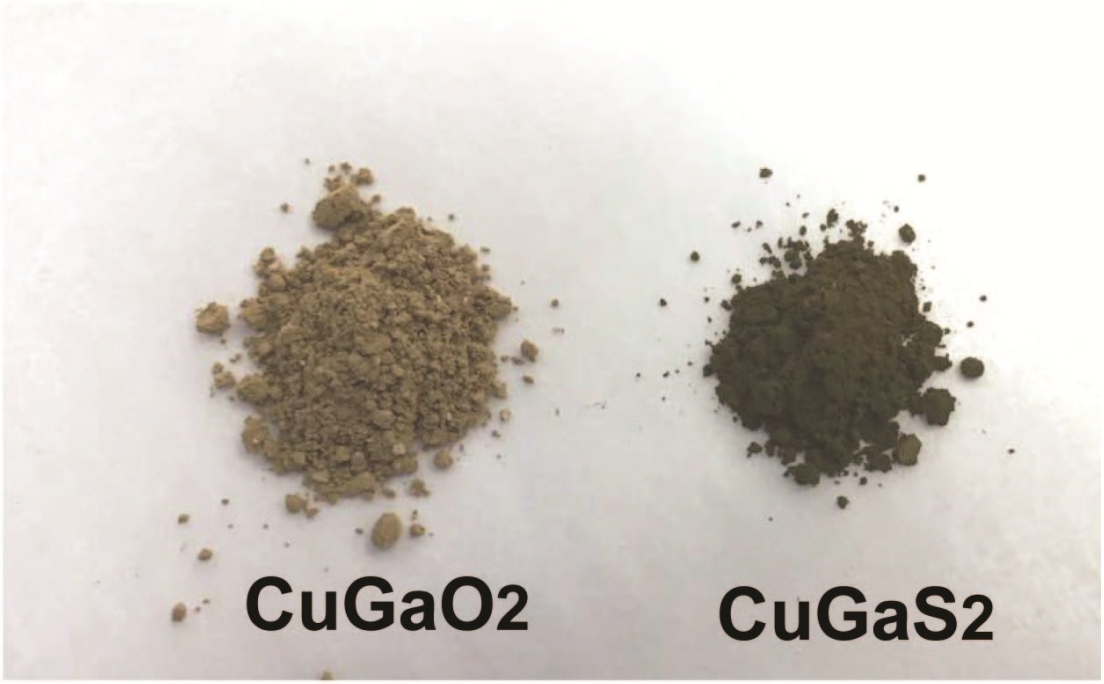

Figure S1. The distinct color of $CuGaO_2$ (brown) and $CuGaS_2$ (dark green) power.

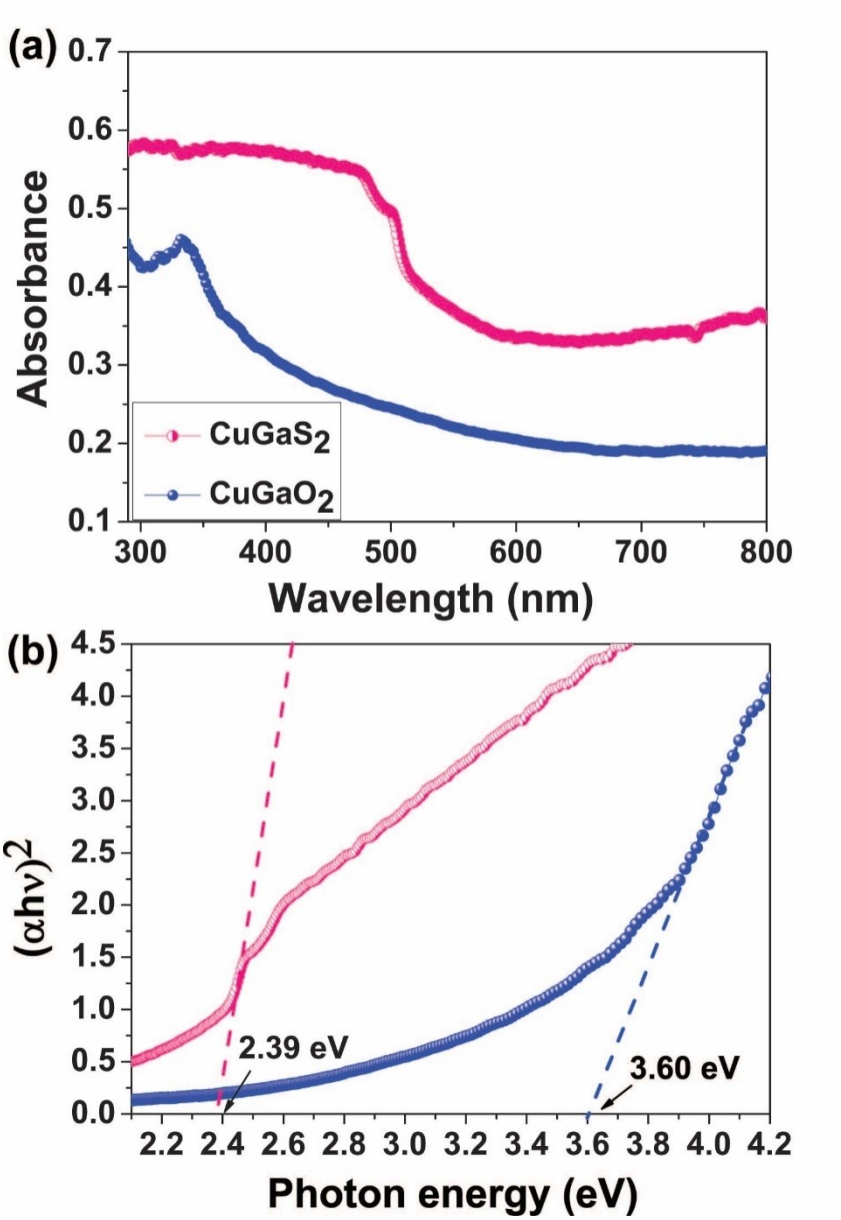

Figure. S2. (a) UV-vis absorption spectra of the$CuGaS_2$ hexagonal nanoplates and $CuGaO_2$ precursor, respectively. (b) The corresponding plot analysis of the optical band gap of $CuGaS_2$ and $CuGaO_2$, respectively.

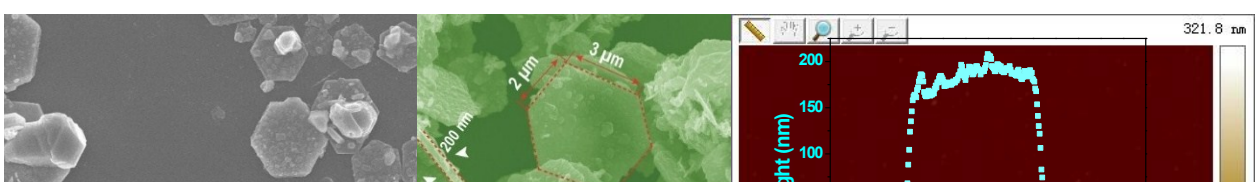

Figure S3. Typical SEM image and AFM image of $CuGaS_2$ hexagonal nanoplates.

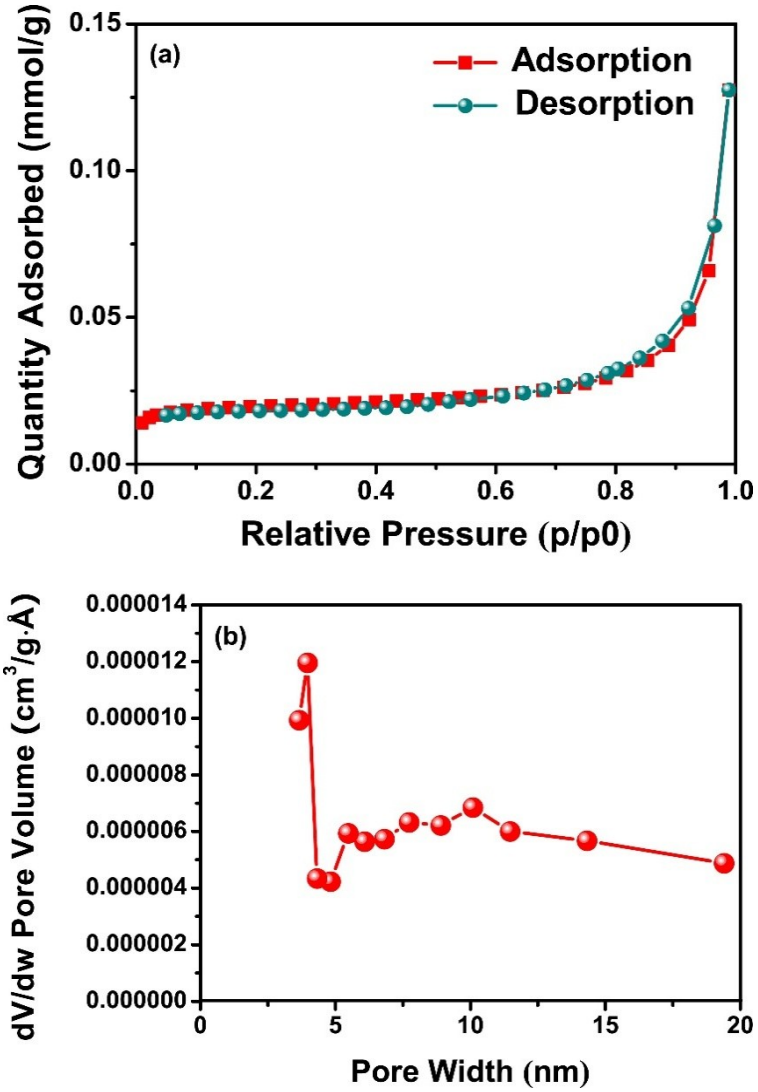

Figure. S4. (a) Nitrogen adsorption–desorption isotherms and (b) pore size distribution of the as-transformed $CuGaS_2$ nanoplates.

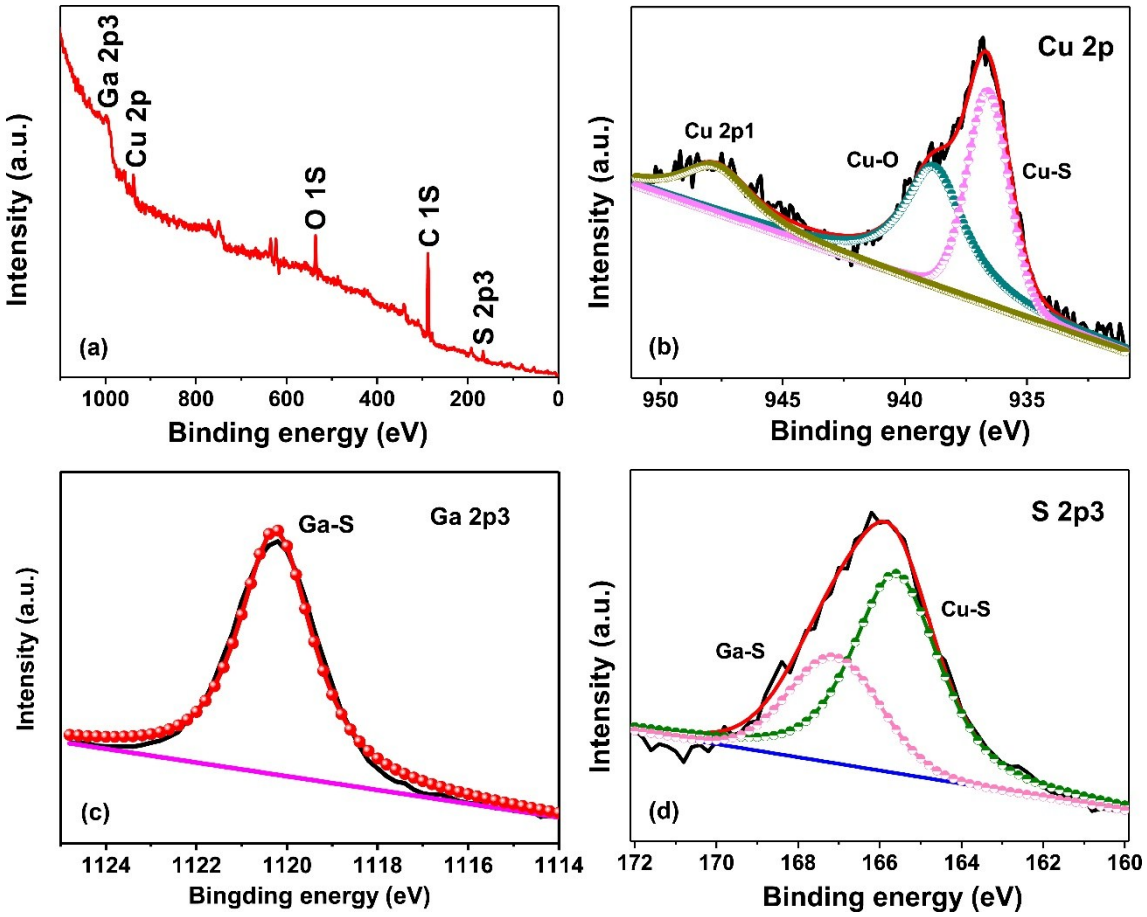

Figure S5. XPS survey spectra and high-resolution XPS spectra of (b) Cu 2p, (c) Ga 2p3 and (d) S 2p3 for our $CuGaS_2$ nanoplates. The full-scan spectra in (a) show the presence of the Cu 2p, Ga 2p and S 2p peaks. The Cu 2p, Ga 2p and S 2p core levels were scanned respectively. As presented in (b), the fitting of Cu 2p spectra disclosed the presence of Cu-S, Cu-OH peaks. The corresponding S 2p3 spectrum of the sample (d) displays three main peaks at 163.1 and 161.5 eV for Ga–S, and Cu–S bonds, respectively.

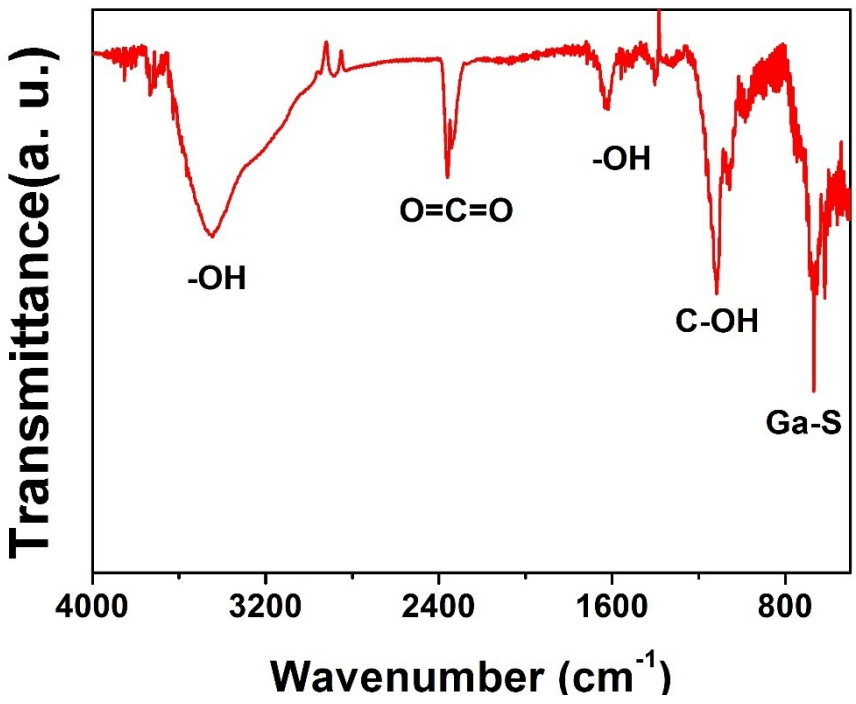

Figure S6. FTIR spectrum for $CuGaS_2$ nanoplates. The large band centered at 3500 cm^{-1} is assigned to the O-H stretching modes of adsorbed water molecules on the sample surface.

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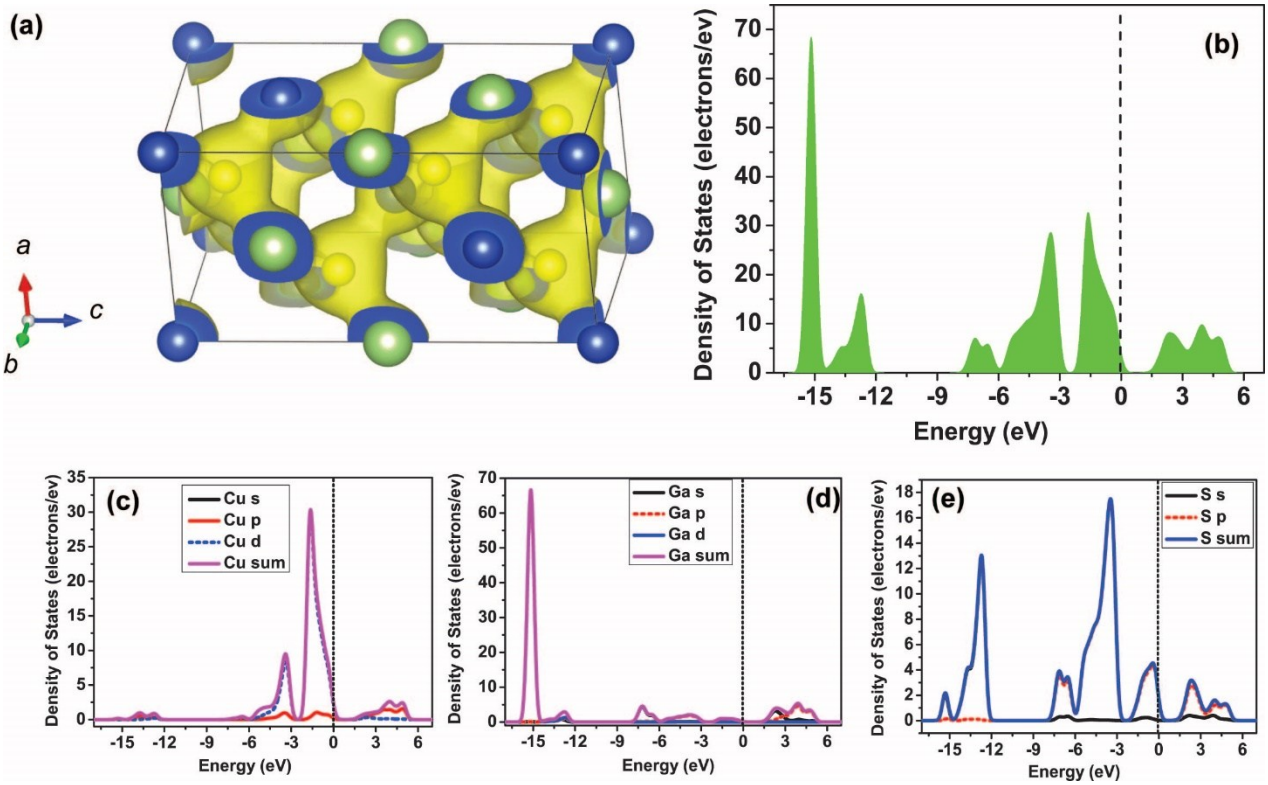

Figure S7. Density function theory calculation studies of $CuGaS_2$. (a) 3D charge density distribution of a $CuGaS_2$unit cell. Blue and yellow regions represent charge accumulation and depletion, respectively. (b) Calculated total density of states (DOS). The projected density of states (PDOS) of (c) Cu s, p, d (d) Ga s, p, d, (e) S s, p orbitals. DFT is hampered by two important shortcomings when applied in this context: (i) the Kohn-Sham (KS) band gap is systematically underestimated by 50% to 100% compared to photoemission experiments; and (ii) there is deficient cancellation of the spurious self-interaction terms in standard functionals, particularly critical for d electrons, which are usually located too high in energy. For systems with shallow d states, like the chalcopyrites, this has a direct effect on the band gap.

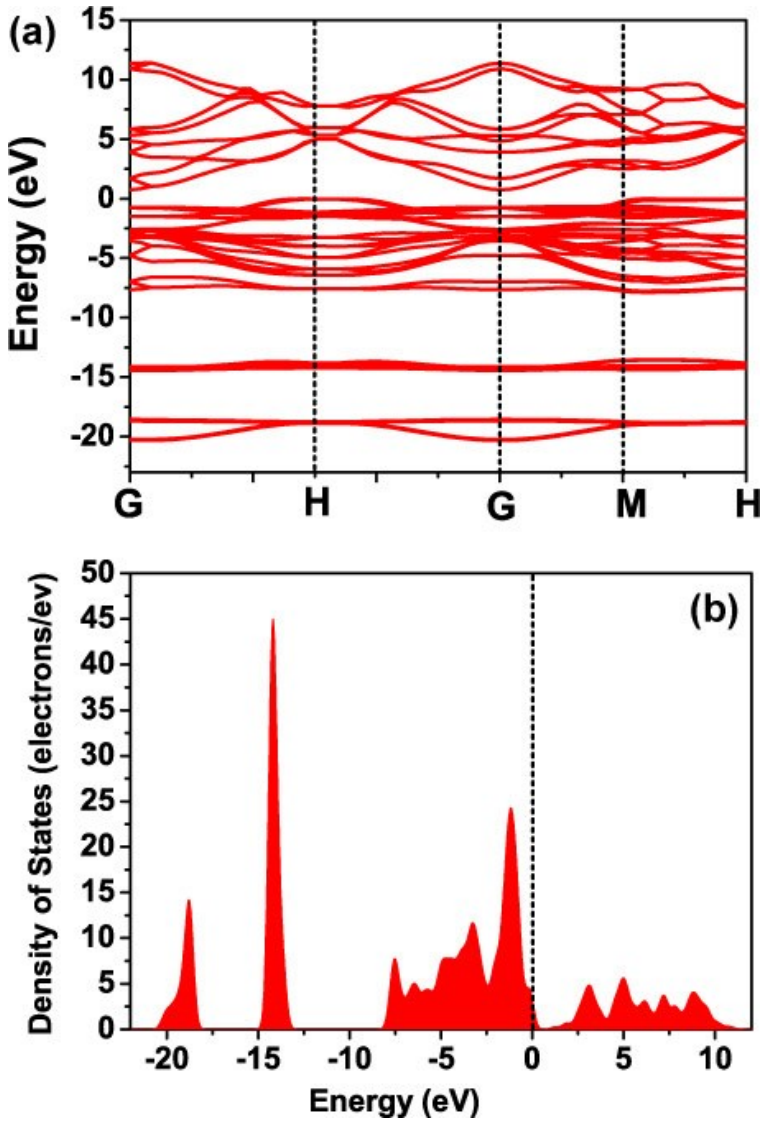

Figure S8. Calculated band structure and (d) total density of states (DOS) of $CuGaO_2$ precursor.

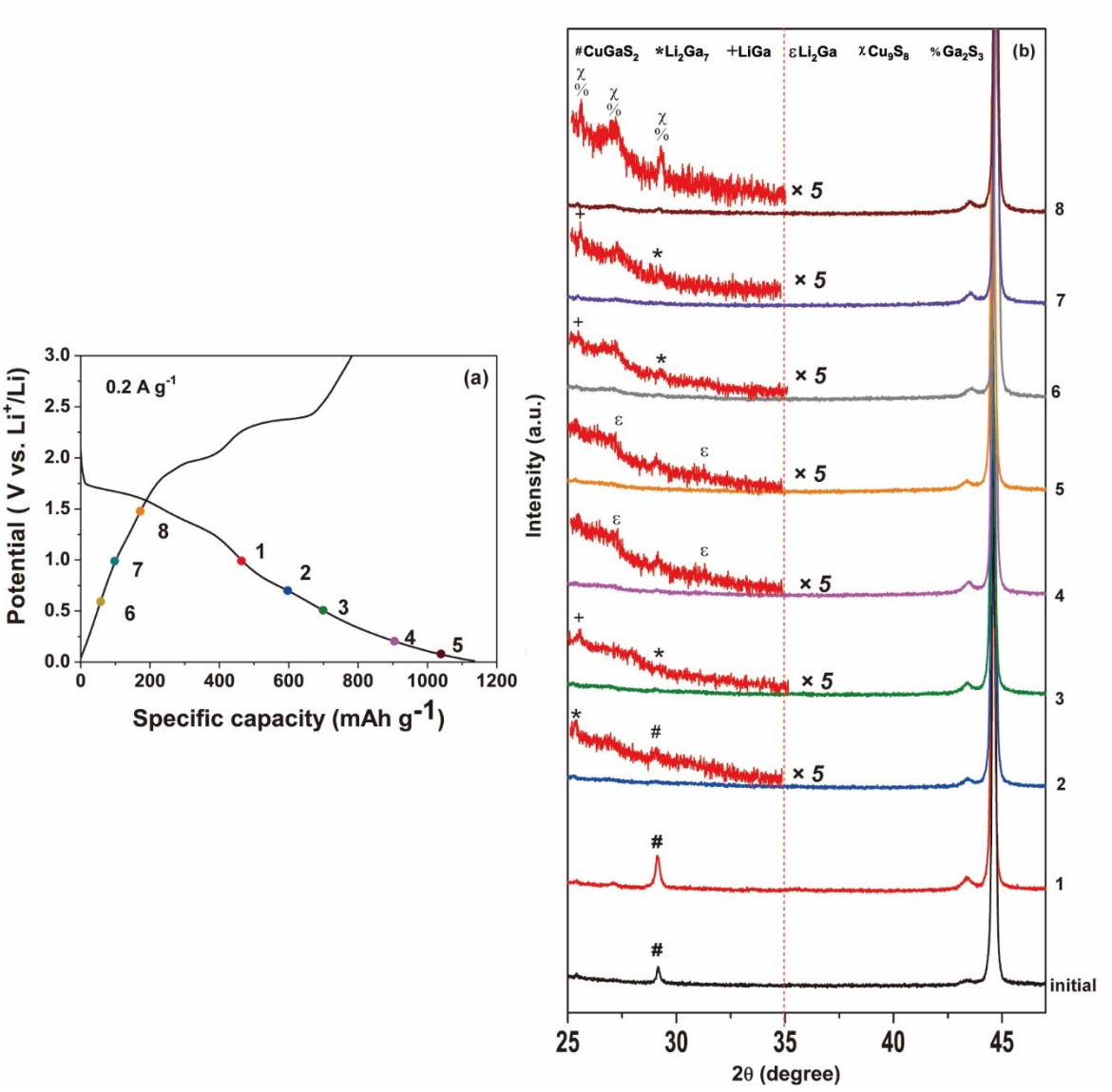

Figure S9. (a) Voltage profile and (b) ex-situ XRD patterns of $CuGaS_2$. (Inset) Enlarged view of the pattern in low angles.

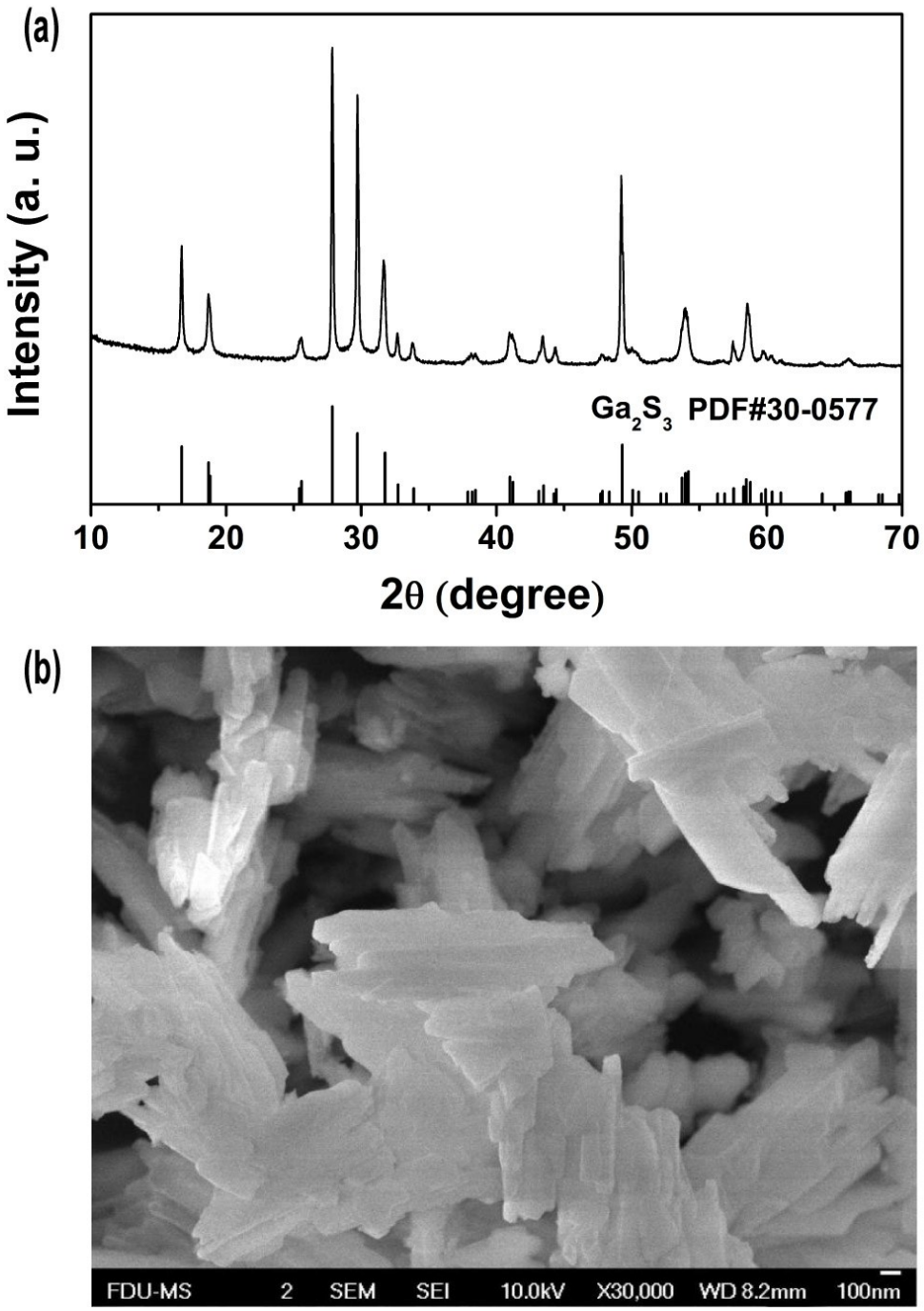

Figure S10. (a) XRD pattern (b) typical SEM image of Ga_2S_3 powder.

Table S1. Comparison of the characteristic parameters of different Ga-based electrodes for LIBs applications.

Electrodes	Current Density	Cycling Number	Specific Capacity/ Temperature	Reference
Ga_2S_3	0.1 A g^{-1}	20	400 mAh g^{-1} @ R.T.	1
Ga_2Se_3	0.1 C	100	600 mAh g^{-1} @ R.T.	2
GaSe	1 A g^{-1}	100	600 mAh g^{-1} @ R.T.	3
	5 A g^{-1}	—	450 mAh g^{-1} @ R.T.	
GaS*x*	0.6 A g^{-1}	100	600 mAh g^{-1} @ R.T.	4
Ga_2O_3	0.05 A g^{-1}	40	800 mAh g^{-1} @ R.T.	5
$CuGaS_2$	**5 A g^{-1}**	**600**	**521 mAh g^{-1} @ R.T**.	**This work**
$CuGaS_2$	**0.5 A g^{-1}**	**80**	**784 mAh g^{-1} @318 K**	**This work**
$CuGaS_2$	**0.5 A g^{-1}**	**80**	**407 mAh g-1 @ 268 K**	**This work**

Table S2. Comparison of the characteristic parameters of different electrodes for NIBs applications.

Electrodes	Current Density	Cycling Number	Specific Capacity	Reference
CoS_2@MWNT	0.1 A g^{-1}	100	568 mAh g^{-1}	6
MoS_2@MWNT	0.05 A g^{-1}	100	504 mAh g^{-1}	7
SnO_2@Al_2O_3	0.134 A g^{-1}	100	375 mAh g^{-1}	8
MoS_2@graphene	0.02 A g^{-1}	100	344 mAh g^{-1}	9
FeS@Carbon	0.5 A g^{-1}	200	280	10
CuS@graphene	1 A g^{-1}	450	345 mAh g^{-1}	11
$CuGaS_2$	**1 A g^{-1}**	**100**	**321 mAh g^{-1}**	**This work**

Reference

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