Tailoring the phase composition of carbon-coated nickel sulfides to achieve a high specific capacitance

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1. Materials Characterization

The crystallographic information, morphology, structure, and phase composition of the as-obtained materials were characterized by powder X-ray diffraction (XRD, PANalytical Empyrean), X-ray photoelectron spectroscopy (XPS, Thermo Scientific K-Alpha), Fourier transform infrared spectroscopy (FTIR, Alpha-P analyzer), scanning electron microscopy (SEM; Zeiss Sigma 300, operated at 3 kV), transmission electron microscopy (TEM; Hitachi HT7700), Raman analysis (WITech Alpha 300R Raman spectrometer with an air-cooled DPSS laser up to 100 mW at 532 nm), thermogravimetric analysis (TGA, Perkin Elmer STA 6000), and BET (N_2 adsorption and desorption isotherms by a Micromeritics at 76 K).

2. Calculation

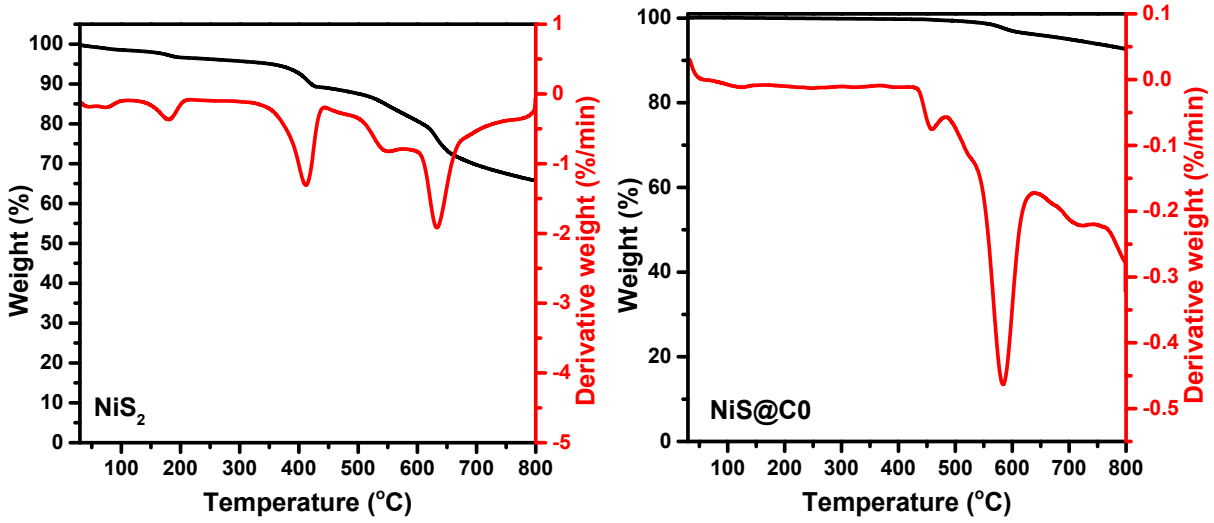
The specific capacitance of the NiS_2, NiS@C0, NiS/NiS_2@C1, and NiS/NiS_2@C2 electrodes was calculated from the GCD curve according to the following equation [1,2]:

$$C_s = \frac{I \times \Delta t}{m \times \Delta V} \tag{S1}$$

where C_s (F/g) is the specific capacitance of the working electrode, I (A) is the discharge current, Δt (s) is the discharge time, m (g) is the mass of the active material in the working electrode, and ΔV (V) is the discharge potential range, respectively.

3. Results

TGA was carried out to evaluate the thermal stability of the as-prepared nickel sulfides including NiS_2, NiS@C0, NiS/NiS_2@C1, and NiS/NiS_2@C2 electrodes. The NiS_2 nanoparticles exhibited a considerable mass loss which may be related to the organic substance (thiourea) attached to the nanoparticles, sulfur elimination or a possible phase transition. The TGA plot for NiS@C0, NiS/NiS_2@C1, and NiS/NiS_2@C2 showed the mass losses which can be related to Ni-S phase transition and elimination of the carbon [3,4].



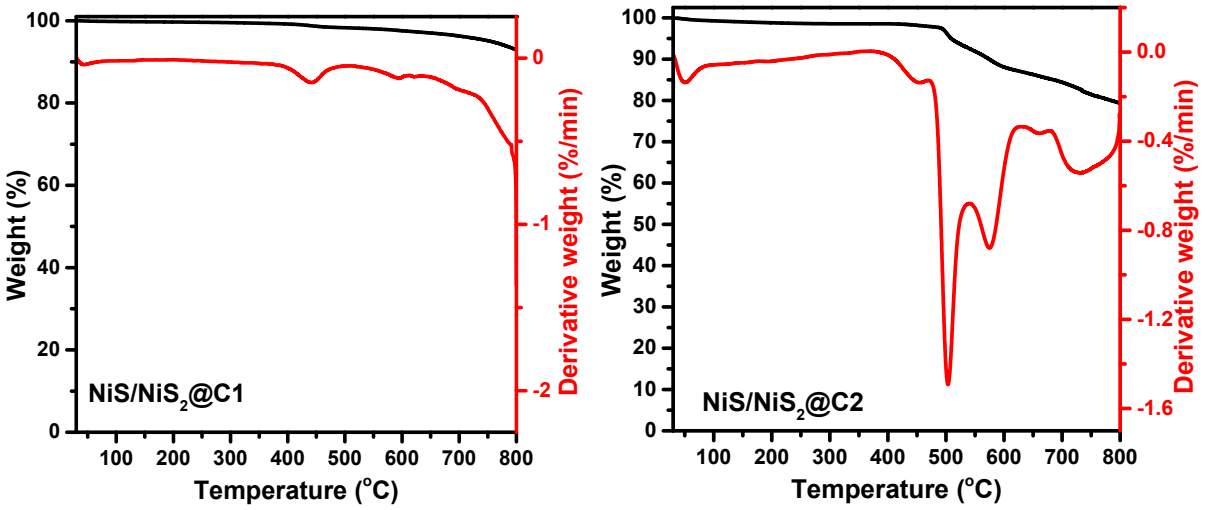


Fig. S1. TGA curves of NiS_2, NiS@C0, NiS/NiS_2@C1, NiS/NiS_2@C2 nanocomposites.

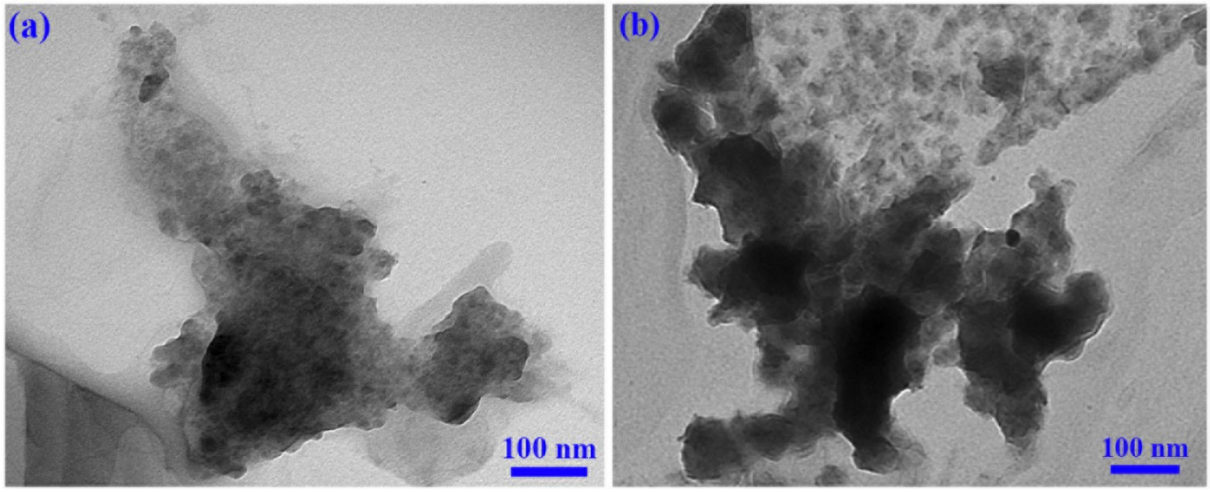


Fig. S2. TEM image of the **(a)** pure NiS_2 and **(b)** NiS_2/NiS@C0 electrode.

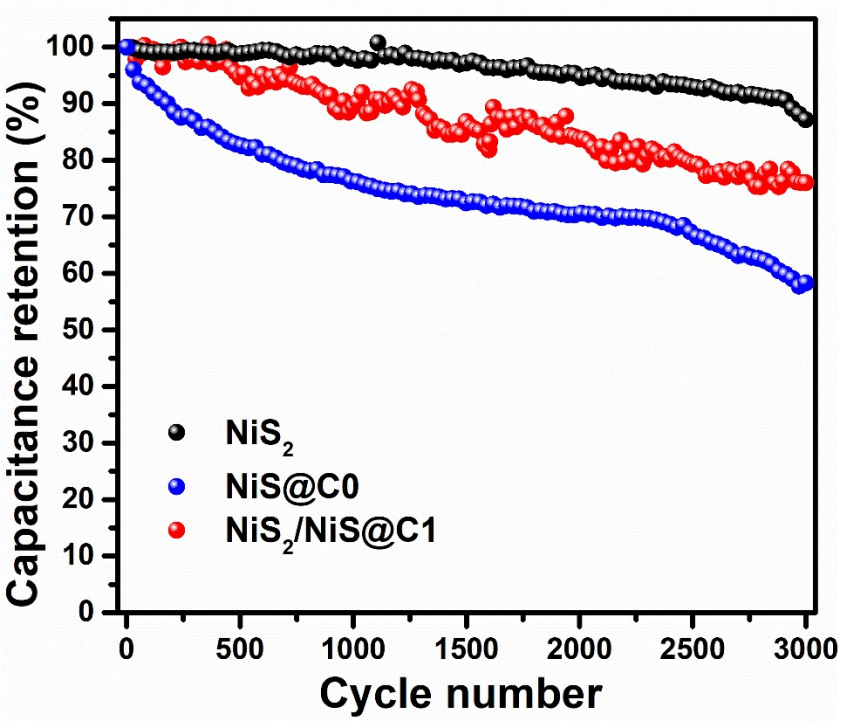


Fig. S3. Cycle stability at 5 A/g of the NiS_2, NiS@C0, and NiS_2/NiS@C1 electrode.

Table S1. XPS data of the NiS_2/NiS@C1 electrode.

Element	Concentration (at. %)	Transition peak	Peak area (counts)	Concentration (at. %)
Ni	5.13	Ni 2p	852.97	26.8
		Ni 2p	855.35	14.7
		Ni 2p	870.27	16.8
		Ni 2p	873.47	16.45
		Ni 2p	859.48	9.8
		Ni 2p	877.38	15.45
S	17.07	S 2p	161.76	49
		S 2p	162.93	35.7
		S 2p	164.00	15.3
C	59.3	C 1s	284.88	92.2
		C 1s	287.6	7.8
O	15.64	O 1s	531.93	100
N	2.86	N 1s	398.47	56.4
		N 1s	400.71	43.6

4. References

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