Electronic Supplementary Information

Hollow CuS nanocube cathode for rechargecharge Mg batteries: Effect of structure on the performance

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Supplementary data: Additional figures and tables as mentioned in the text

1. Lab-made cell for the Mg battery test

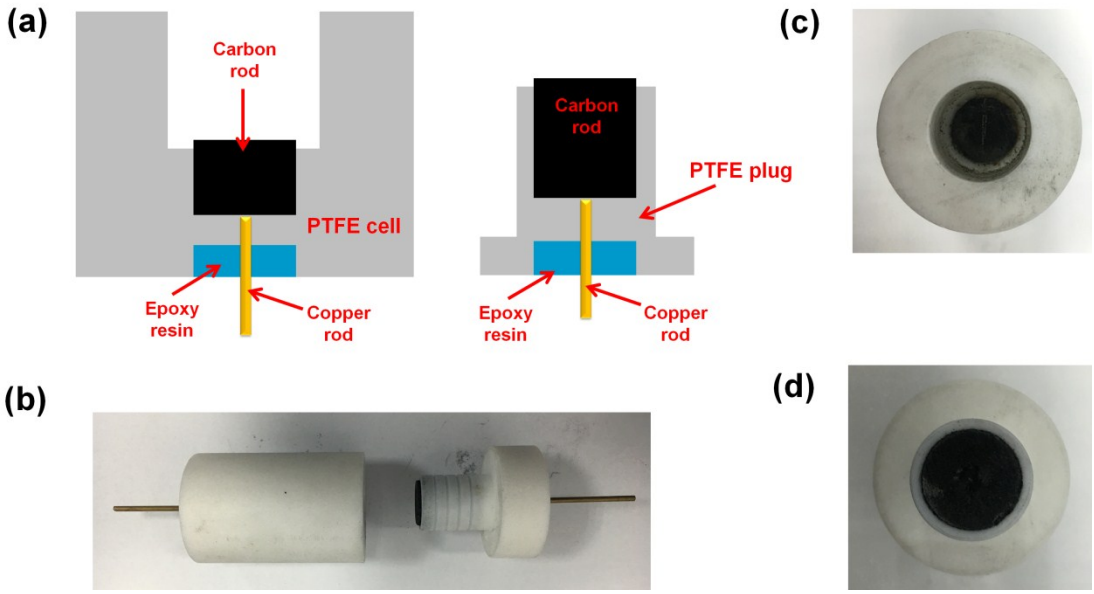
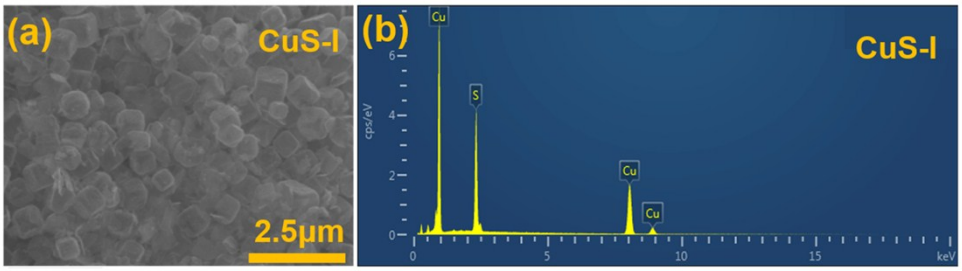


Fig. S1 (a) Schematic drawing and (b, c, d) photos of the lab-made PTFE cell used for Mg battery tests. The cell is made of customer-designed PTFE cell body and carbon rod electrode (with a copper rod inserted in). Epoxy resin is used to fix the carbon electrode and seal the crack. PTFE tape is used for the sealing during the Mg cell fabrication.

2. Appearance comparison

Fig. S2 Hollow CuS nanocube (left) and commercial CuS (right) with the same mass.

3. EDX spectra of CuS-I



(c)

Element	Weight%	Atomic%
Cu	73.40	58.20
S	26.6	41.80
Total	100	100

Fig. S3 SEM image and EDX spectra

4. XPS spectra

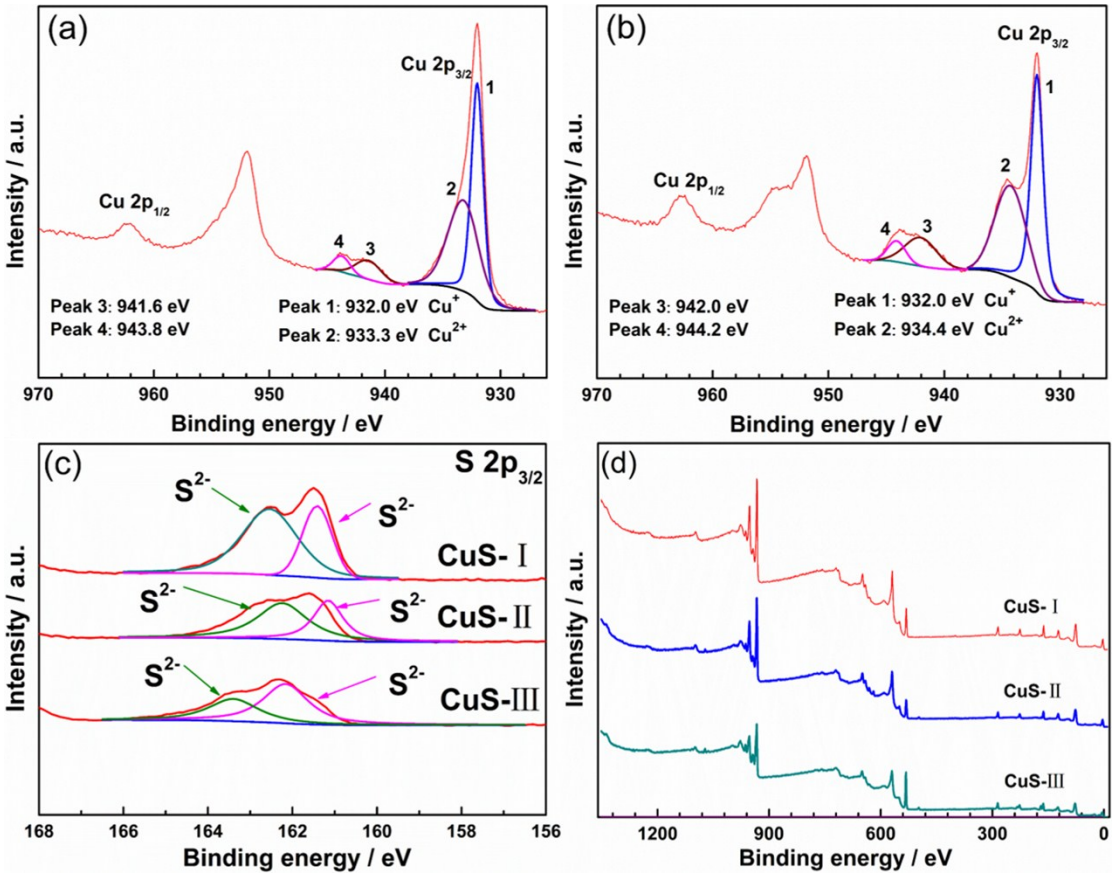


Fig. S4 XPS spectra (Cu 2p) of (a) CuS-II and (b) CuS-III, (c) S 2p spectra, and (d) full spectra.

5. The charge/discharge curves and cycling performance of carbon cloth

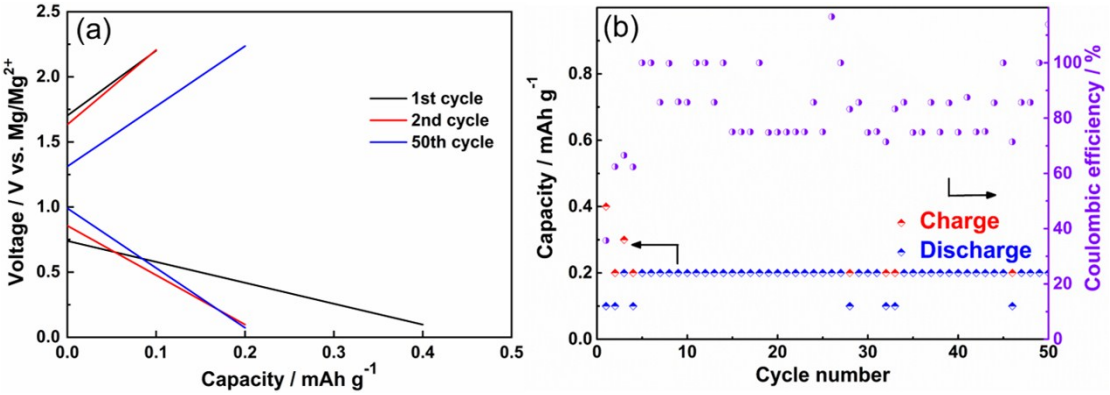


Fig. S5 The charge/discharge curves and cycling performance of carbon cloth.

6. Rate performance

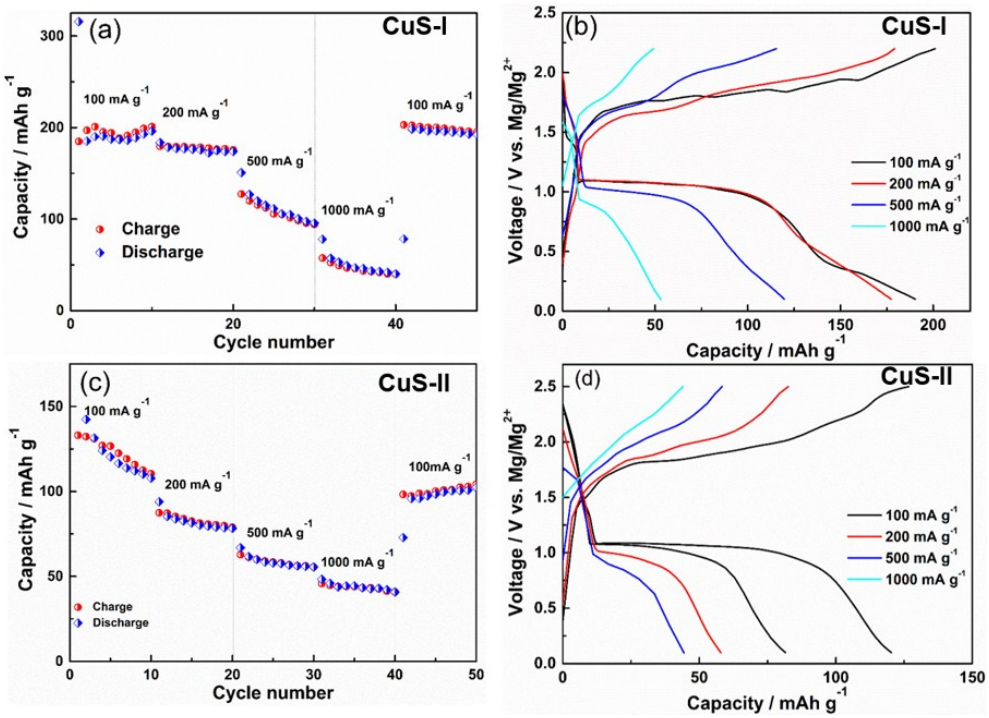


Fig. S6 Rate performance of CuS-I and CuS-II.

7. CV curves of CuS-II and CuS-III electrodes

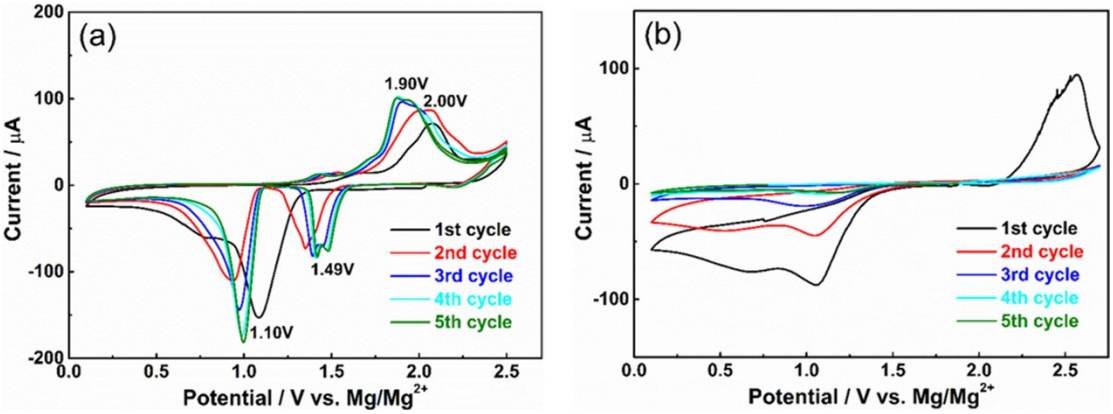


Fig. S7 CV curves of CuS-II and CuS-III electrodes

8. Determination of Mg^{2+} diffusion coefficient for CuS-I and CuS-II

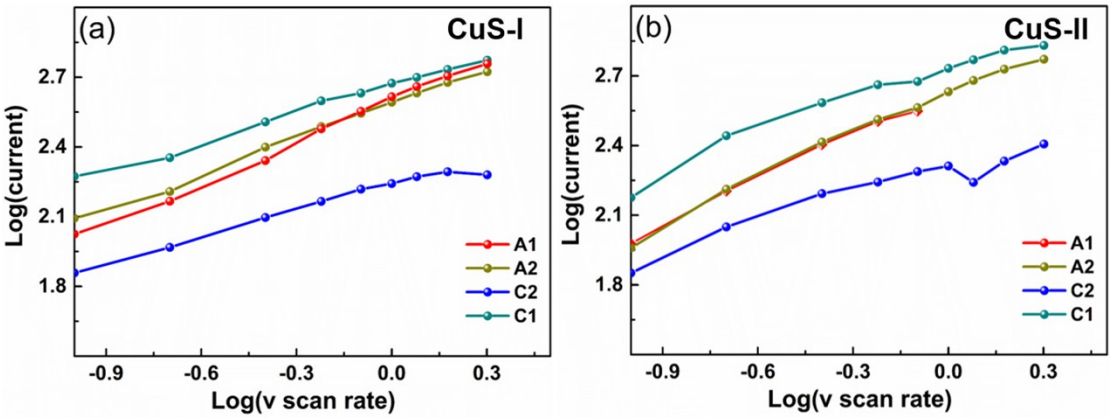


Fig. S8 Log(*i*) vs. log(*v*) plots for different redox peaks of CuS-I and CuS-II electrodes.

Table S1 Calculation of Mg^{2+} diffusion coefficients

	CuS-I		CuS-II	
peak	$i_p/v^{1/2}$	D ($\times10^{-9}$ cm^2 s^{-1})	$i_p/v^{1/2}$	D ($\times10^{-9}$ cm^2 s^{-1})
C2	–0.1193	8.158	–0.1479	5.571
C1	–0.3825	83.86	–0.4726	56.89
A2	0.3816	83.47	0.4595	53.77
A1	0.4475	114.8	0.3999	40.73

The diffusion coefficient of Mg^{2+} is calculated by the following equation:

$$i_p=2.69\times10^5 n^{3/2} A D^{1/2} v^{1/2} C_0$$

where i_p is the peak current (A), n is the number of electrons per molecule during the reaction, A is the contact area between the electrode and electrolyte, D is the diffusion coefficient of Mg^{2+} (cm^2 s^{-1}), C_0 is the concentration of Mg^{2+} ion in the electrode material, and v is the scan rate (V s^{-1}).