

Electronic Supplementary Information

Mg-storage properties of hollow copper selenide nanocubes

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

1. Full XPS spectra.

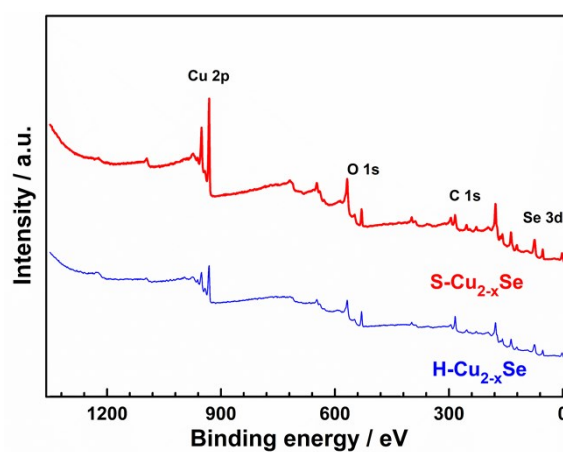


Fig. S1 Full XPS spectra of H-Cu_{2-x}Se and S-Cu_{2-x}Se.

2. Rate capability of S-Cu_{2-x}Se.

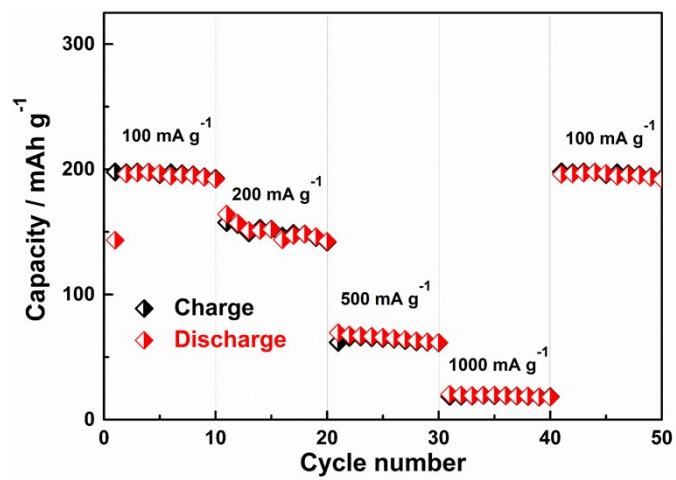


Fig. S2 Rate capability of S-Cu_{2-x}Se at different current densities from 100 to 1000 mA g⁻¹. The test started from an activated S-Cu_{2-x}Se.

3. Charge/discharge curves for the rate performance

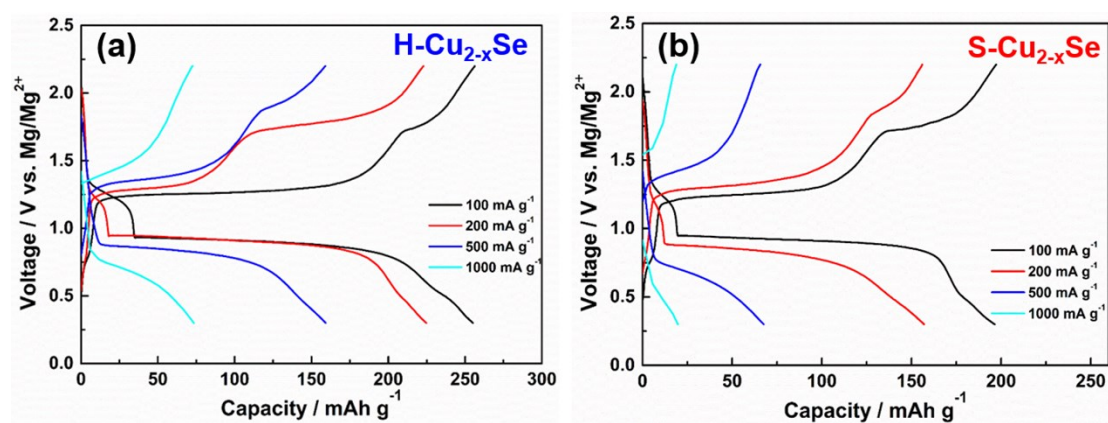


Fig. S3 Charge/discharge curves for rate performance of (a) H-Cu_{2-x}Se and (b) S-Cu_{2-x}Se.

4. Determination of Mg^{2+} diffusion coefficients for $\text{H-Cu}_{2-x}\text{Se}$ and $\text{S-Cu}_{2-x}\text{Se}$.

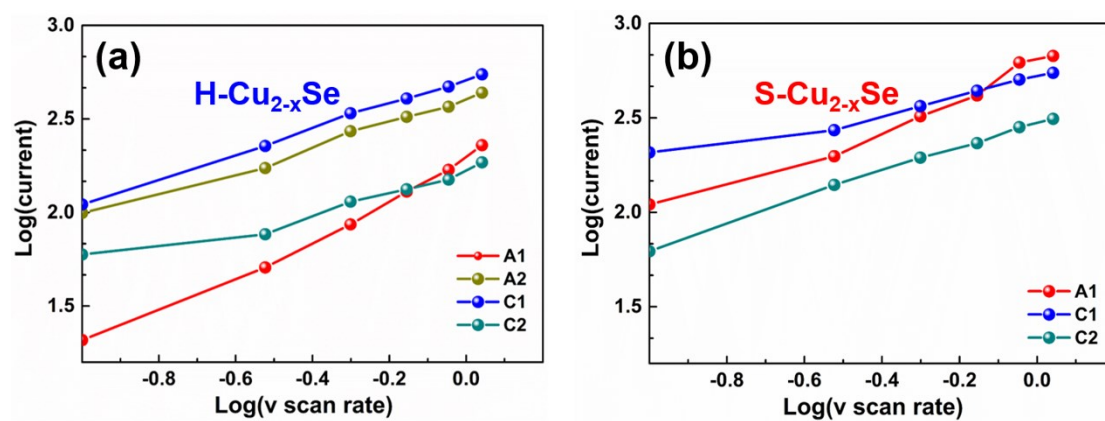


Fig. S4 $\text{Log}(i)$ vs. $\text{log}(v)$ plots for different redox peaks of $\text{H-Cu}_{2-x}\text{Se}$ and $\text{S-Cu}_{2-x}\text{Se}$ electrodes.

Table S1 Calculation of Mg²⁺ diffusion coefficients

peak	H-Cu _{2-x} Se		S-Cu _{2-x} Se	
	$i_p/v^{1/2}$	$D (\times 10^{-9} \text{ cm}^2 \text{ s}^{-1})$	$i_p/v^{1/2}$	$D (\times 10^{-10} \text{ cm}^2 \text{ s}^{-1})$
A1	0.2764	4.3124	0.8086	16.4032
A2	0.4609	11.9911	/	/
C2	-0.1693	1.6179	-0.3429	2.9498
C1	-0.5940	19.9167	-0.4871	5.9525

The diffusion coefficient of Mg²⁺ is calculated by the following equation:

$$i_p = 2.69 \times 10^5 n^{3/2} A D^{1/2} v^{1/2} C_0$$

where i_p is the peak current (A), n is the number of electrons per molecule during the reaction, A (cm²) is the contact area between the electrode and electrolyte, D is the diffusion coefficient of Mg²⁺ (cm² s⁻¹), C_0 (mol cm⁻³) is the concentration of Mg²⁺ ion in the electrode material, and v is the scan rate (V s⁻¹).