

Supporting information:

Highly defective and conductive Cu-doped 1T/2H-MoS₂ nanosheets as high-capacity cathode materials for enhanced magnesium ion storage

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Ao Xu, and Yan Liu were the co-first authors in this work.

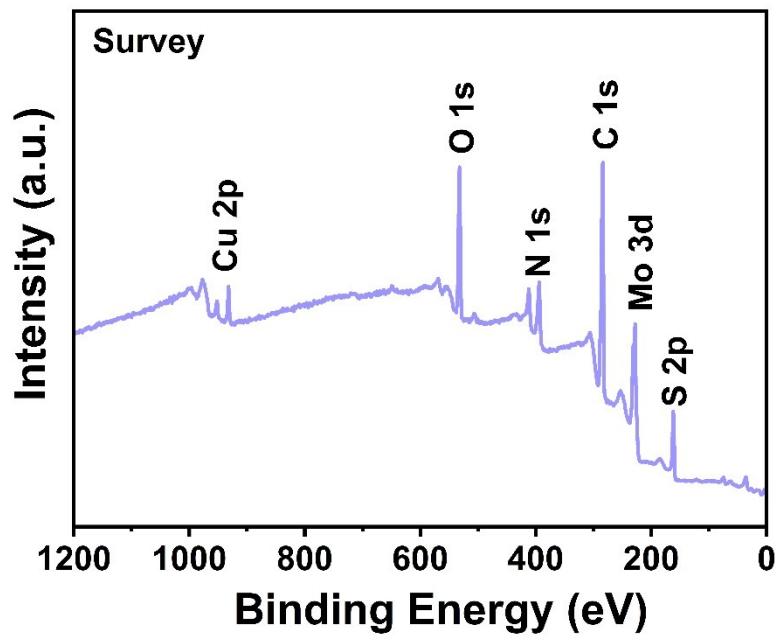


Fig. S1 XPS survey spectrum of Cu-MoS₂-2.

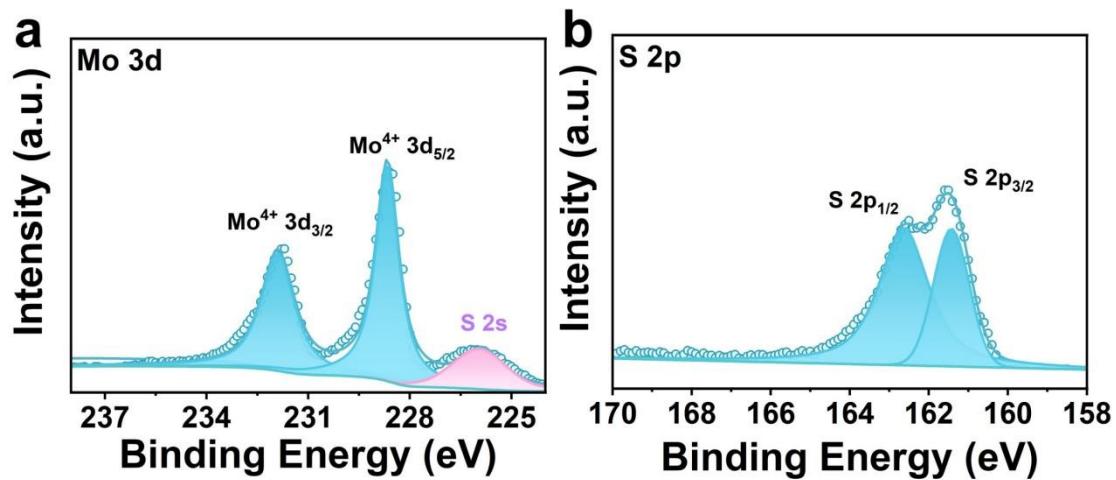


Fig. S2 XPS survey spectrum of MoS₂.

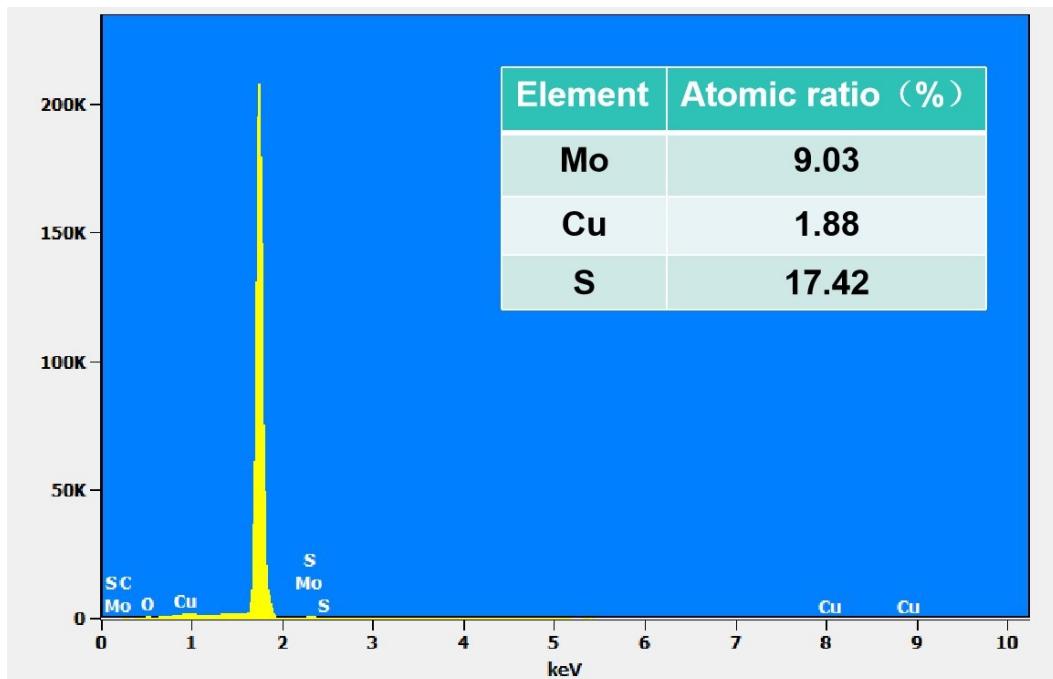


Fig. S3 EDS spectrum of Cu-MoS₂-2.

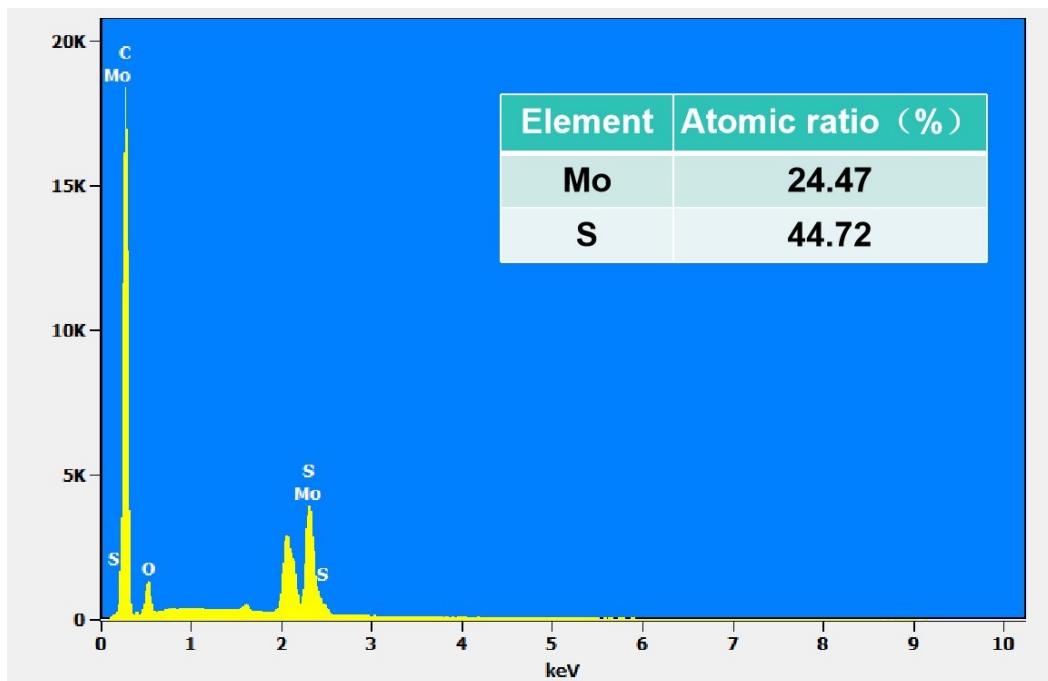


Fig. S4 EDS spectrum of MoS₂.

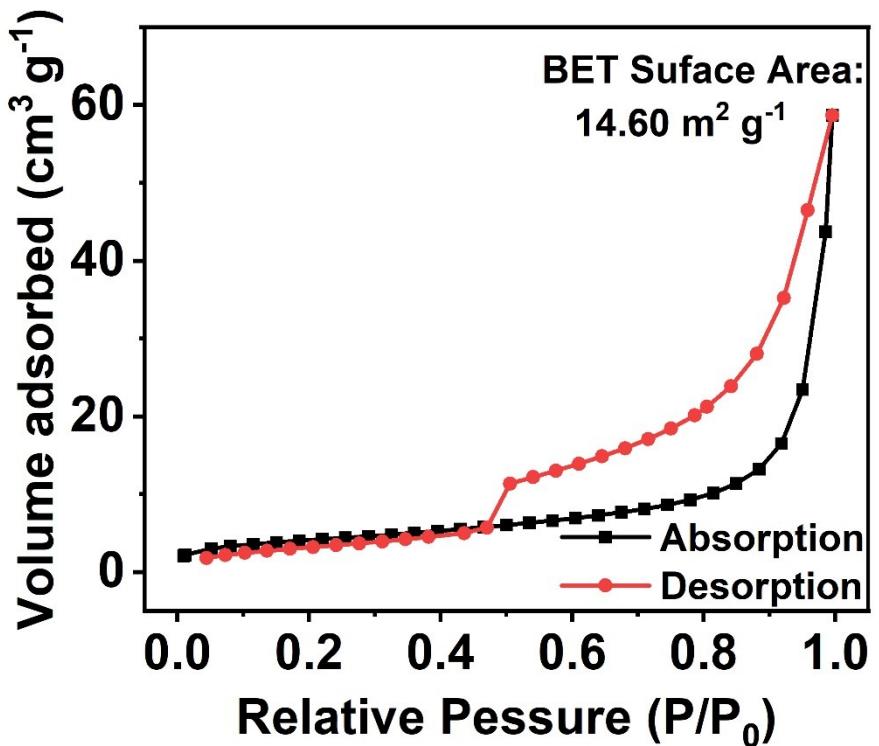


Fig. S5 Nitrogen isothermal adsorption/desorption curves of Cu-MoS₂-2.

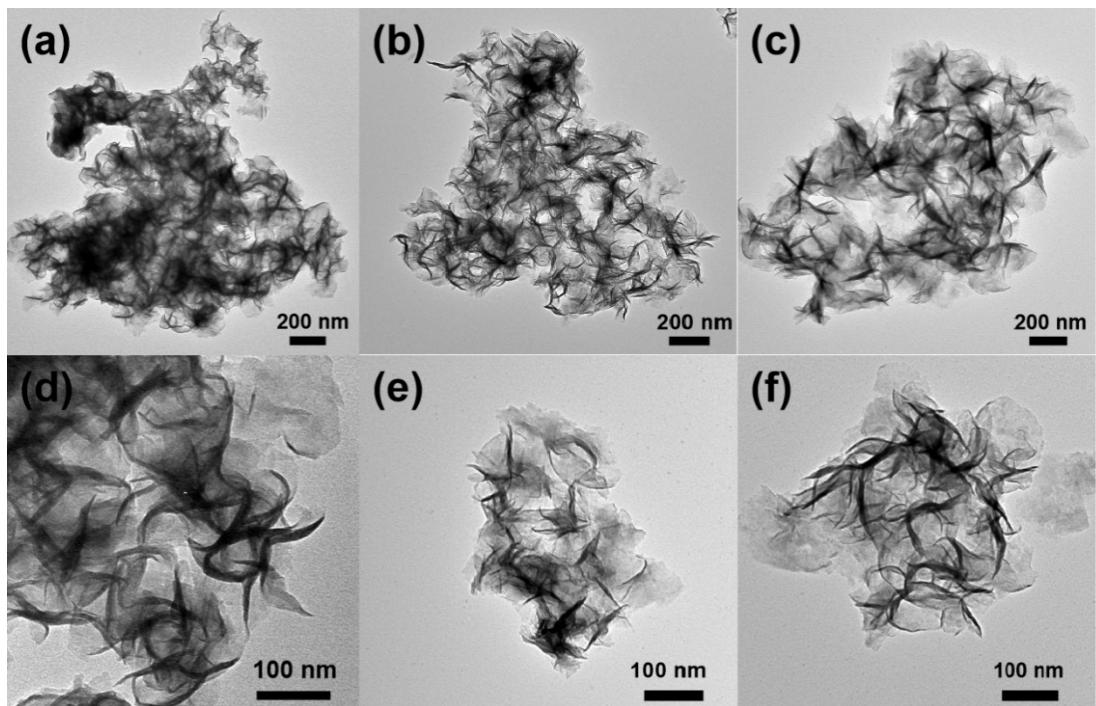


Fig. S6 TEM images of (a-d) MoS₂, (b-e) Cu-MoS₂-1, and (c-f) Cu-MoS₂-3.

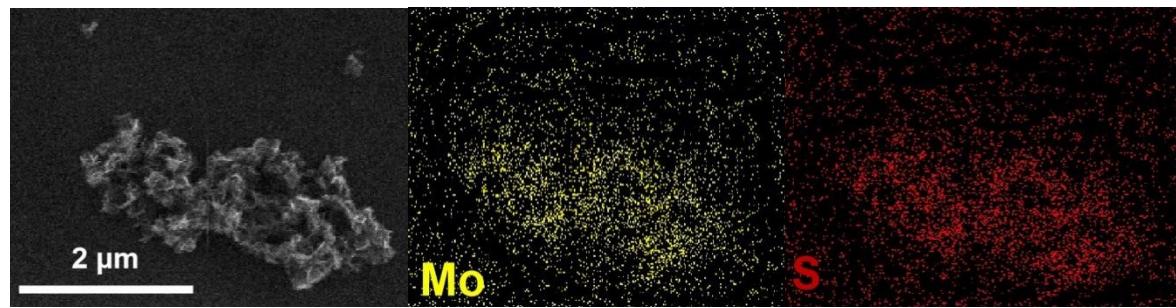


Fig. S7 EDS elemental mappings of MoS_2 .

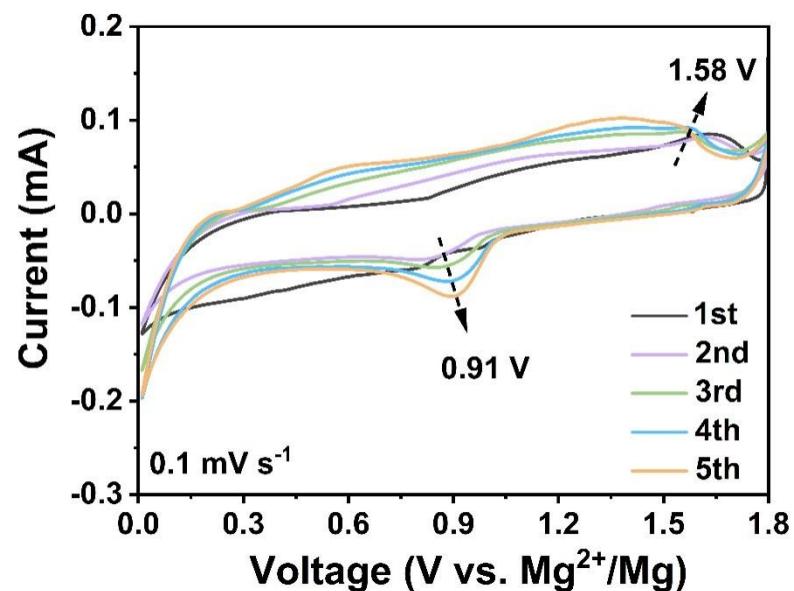


Fig. S8 CV curves of MoS_2 for the first five cycles.

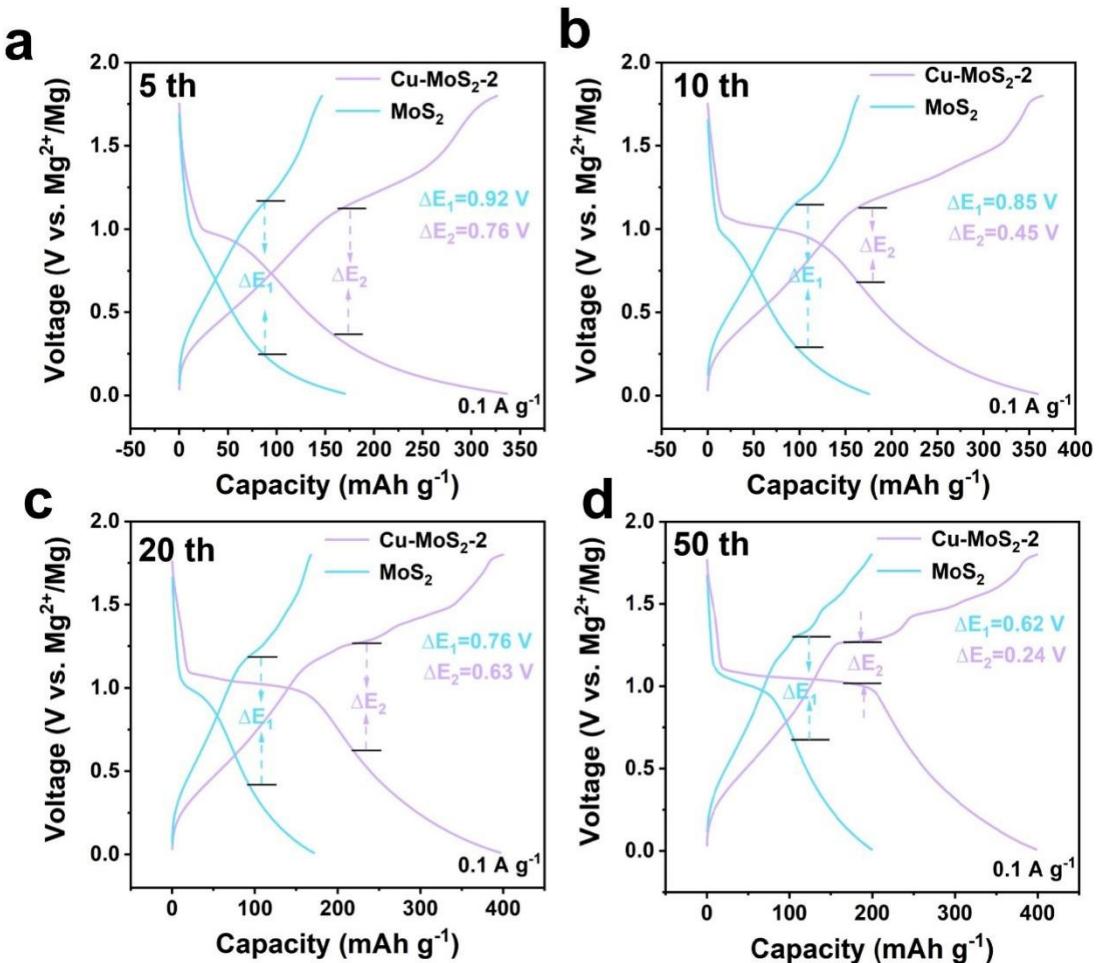


Fig. S9 (a-d) Discharge/charge profiles for different cycles at 0.1 A g⁻¹ of Cu-MoS₂-2 and MoS₂.

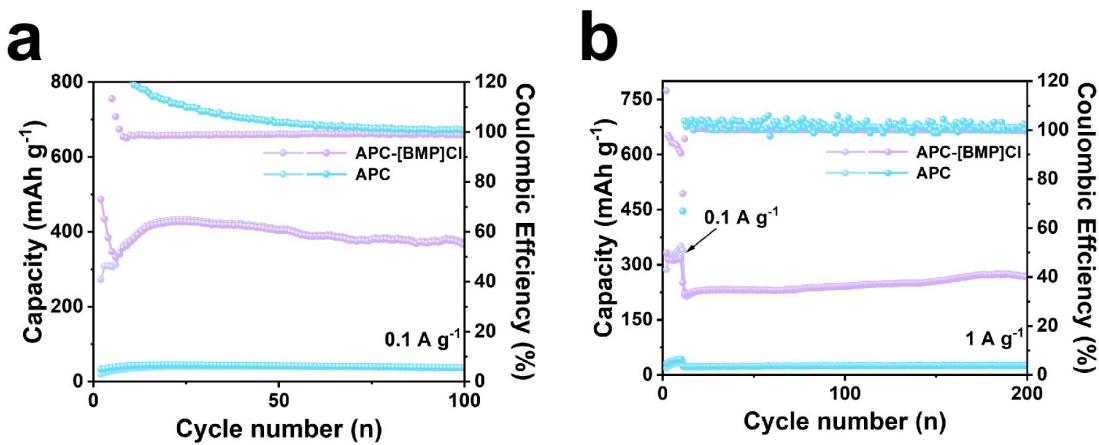


Fig. S10 Cyclic performances of Cu-MoS₂-2 in APC and APC-[BMP]Cl electrolytes:
(a) 0.1 A g⁻¹, and (b) 1.0 A g⁻¹.

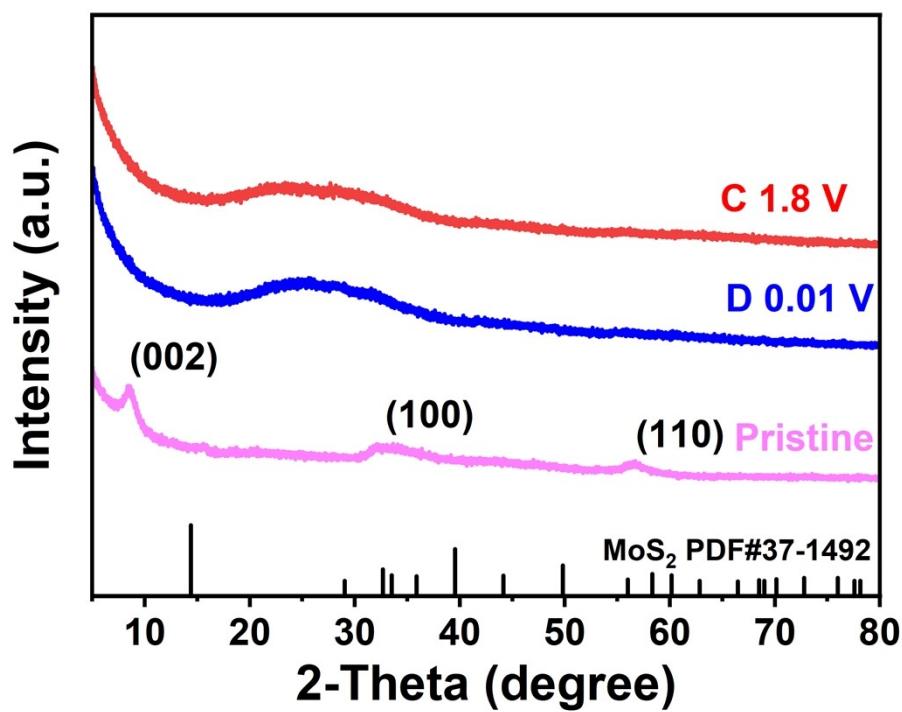


Fig. S11 *Ex-situ* XRD patterns of Cu-MoS₂-2 at different discharge/charge states.

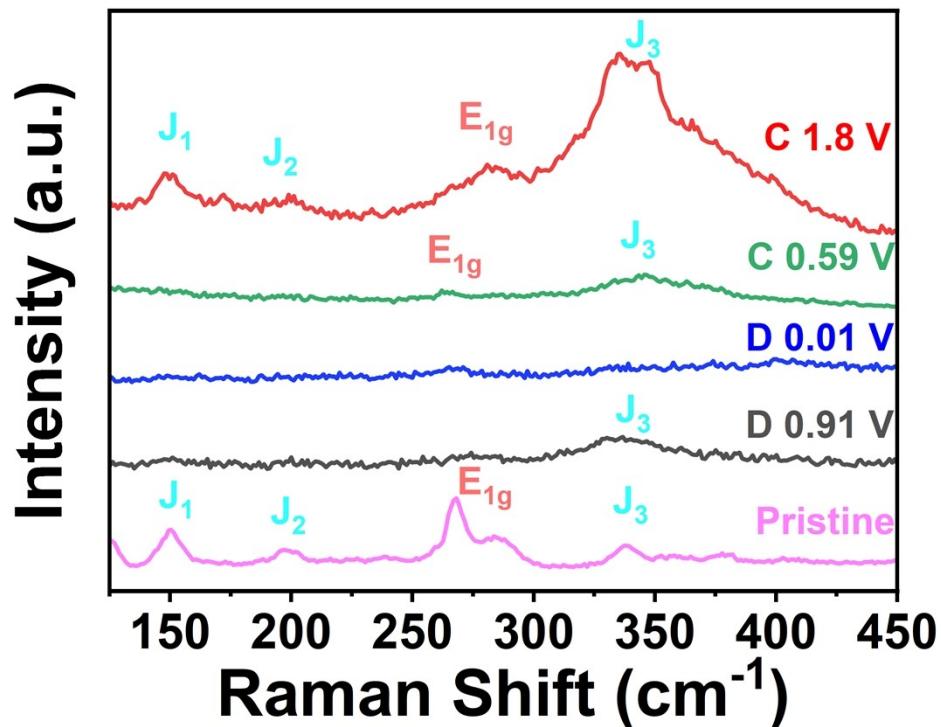


Fig. S12 *Ex-situ* Raman spectra of Cu-MoS₂-2 at different discharge/charge states.

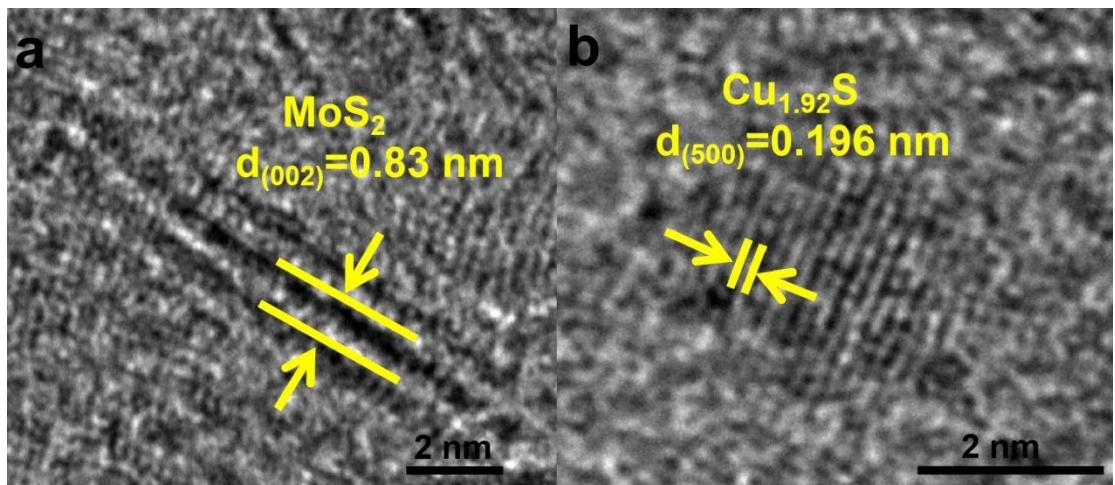


Fig. S13 (a) and (b) HRTEM images of Cu-MoS₂-2 after charging to 1.8 V.

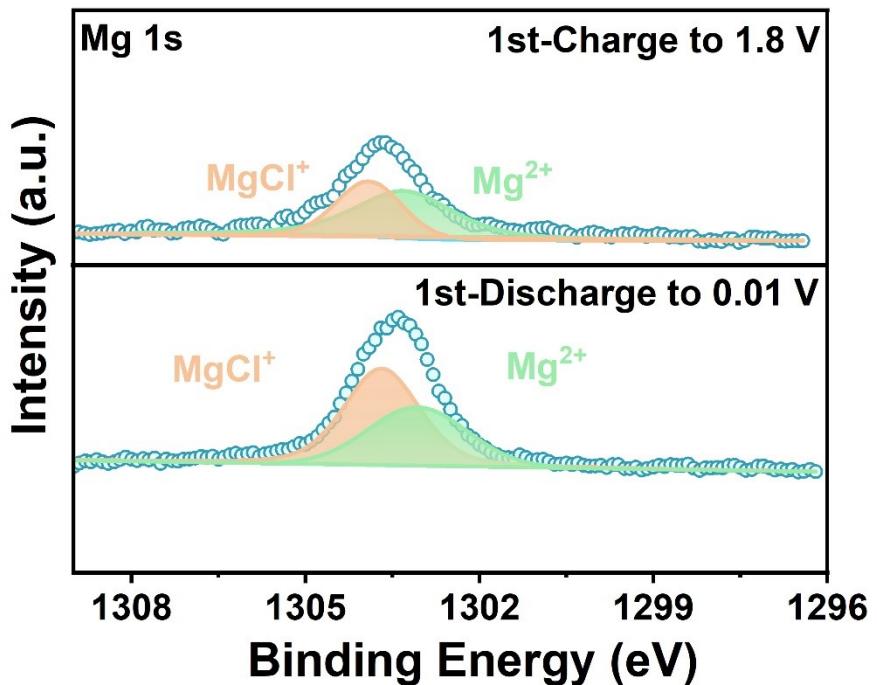


Fig. S14 *Ex-situ* XPS spectra of Mg 1s.

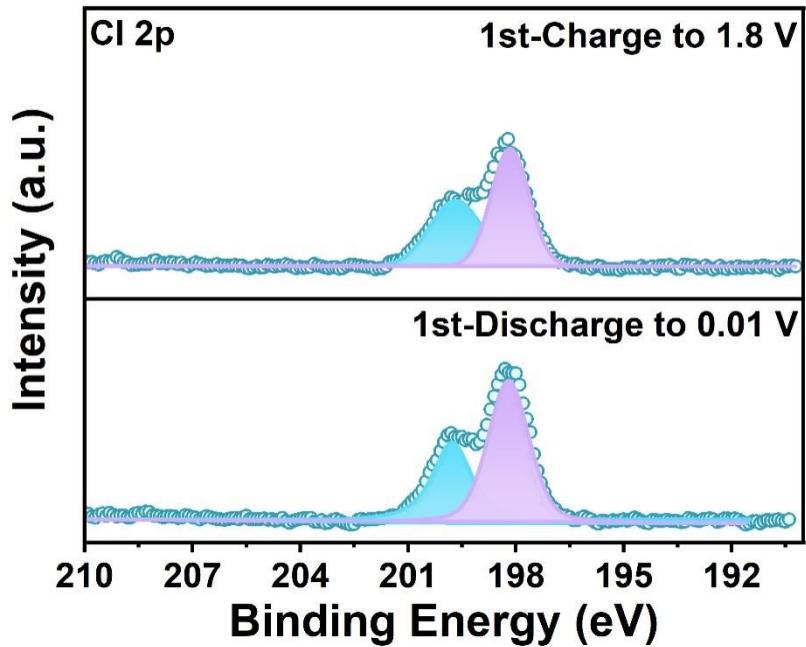


Fig. S15 *Ex-situ* XPS spectra of Cl 2p.

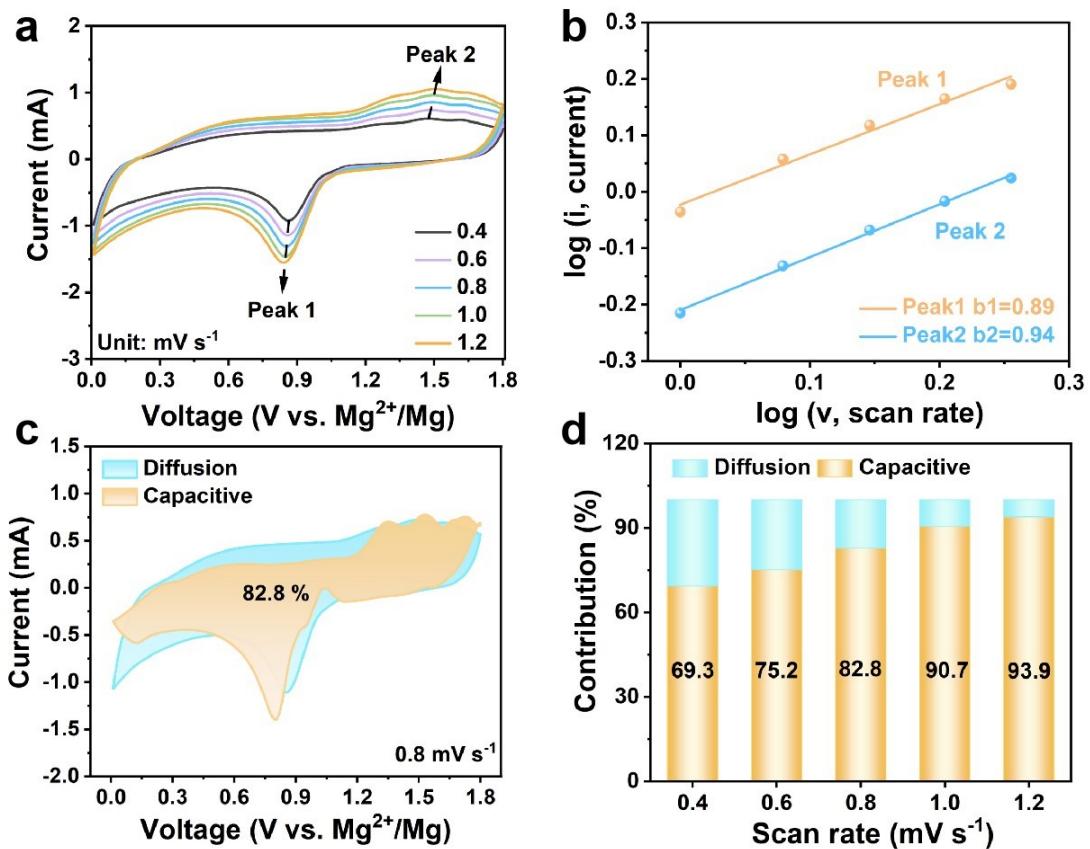


Fig. S16 Kinetic analysis of MoS₂: (a) CV curves at different scan rates, (b) b values obtained from $\log i$ versus $\log v$, (c) percentage of capacitive contributions at 0.8 mV s^{-1} , (d) percentage of capacitive contributions at different scan rates.

Table S1 Electric conductivity data at different pressures of MoS₂ and Cu-MoS₂-2 via the four probe method.

| Electrode materials | Height (mm) | Pressure (Mpa) | Temperature (°C) | Humidness (%RH) | Electric conductivity (S m ⁻¹) |
|-----------------------------|-------------|----------------|------------------|-----------------|--|
| MoS₂ | 0.94 | 18.3 | 25 | 50 | 0.0077 |
| | 0.97 | 16.07 | 25 | 50 | 0.0070 |
| | 0.98 | 14.07 | 25 | 50 | 0.0049 |
| | 1 | 12.07 | 25 | 50 | 0.0042 |
| | 1.04 | 10.17 | 25 | 50 | 0.0037 |
| | 1.07 | 8 | 25 | 50 | 0.0031 |
| | 1.1 | 6.11 | 25 | 50 | 0.0026 |
| | 1.12 | 4.3 | 25 | 50 | 0.0022 |
| | 1.14 | 2.24 | 25 | 50 | 0.0018 |
| | 0.88 | 18.25 | 25 | 50 | 1.6667 |
| Cu-MoS₂-2 | 0.96 | 16.12 | 25 | 50 | 1.3736 |
| | 0.97 | 14.28 | 25 | 50 | 1.1990 |
| | 0.98 | 12.45 | 25 | 50 | 1.0330 |
| | 1 | 10.24 | 25 | 50 | 0.4545 |
| | 1.03 | 8.33 | 25 | 50 | 0.1852 |
| | 1.16 | 6.06 | 25 | 50 | 0.0980 |
| | 1.21 | 4.22 | 25 | 50 | 0.0390 |
| | 1.29 | 2.34 | 25 | 50 | 0.0128 |

Table S2 Reaction impedance derived from EIS spectra.

| Electrode materials | $R_s (\Omega)$ | $R_{SEI} (\Omega)$ | $R_{ct} (\Omega)$ |
|-----------------------------|----------------|--------------------|-------------------|
| MoS₂ | 26.68 | 18.93 | 28.17 |
| Cu-MoS₂-1 | 19.38 | 15.91 | 26.66 |
| Cu-MoS₂-2 | 18.36 | 11.17 | 26.38 |
| Cu-MoS₂-3 | 19.21 | 12.41 | 25.66 |

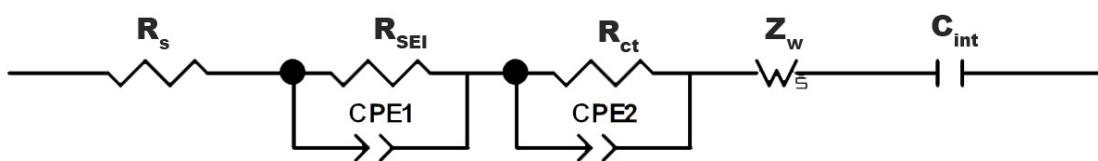


Fig. S17 Diagram of equivalent circuit.