

Investigating Li-S Electro-Crystallisation Mechanisms through Synchrotron Wide Angle X-ray Scattering of Carbon-Sphere Hosts.

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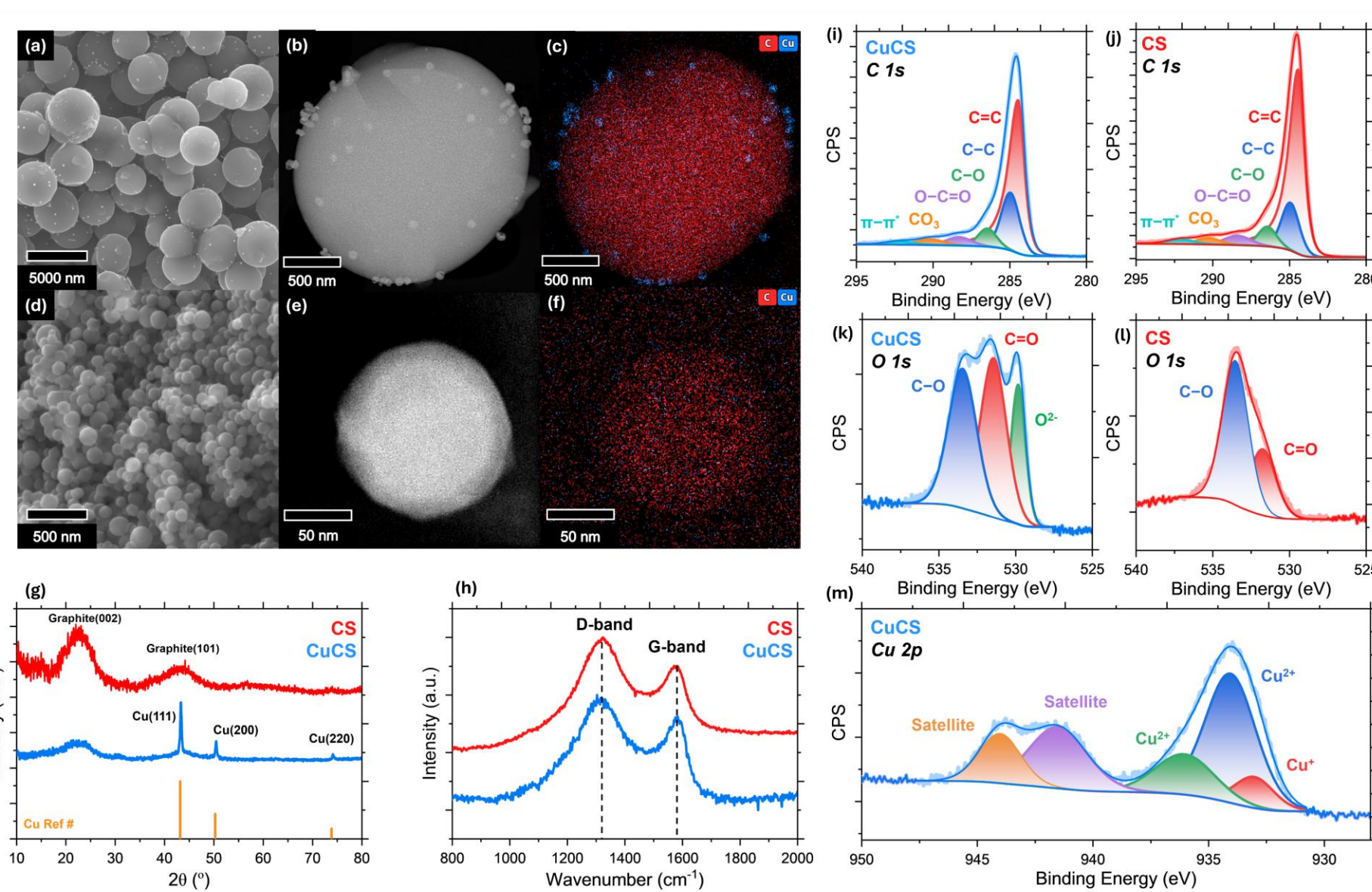
INTRODUCTION



Conversion-type electrodes will play a crucial role in “beyond Li-ion” battery technologies and are essential for facilitating increasing energy storage demands. Among these, **lithium-sulfur (Li-S) batteries** stand out due to their **high theoretical specific charge** (1672 mAh g⁻¹) and **abundant supply of raw materials**.

In this study, we develop a novel sulfur host material, **copper nanoparticle decorated carbon spheres (CuCS)**, synthesised through the facile hydrothermal carbonisation of glucose. Using *operando* synchrotron wide angle X-ray scattering (WAXS), we **probe the real-time structural evolution** of sulfur species during battery cycling.

CHARACTERISATION



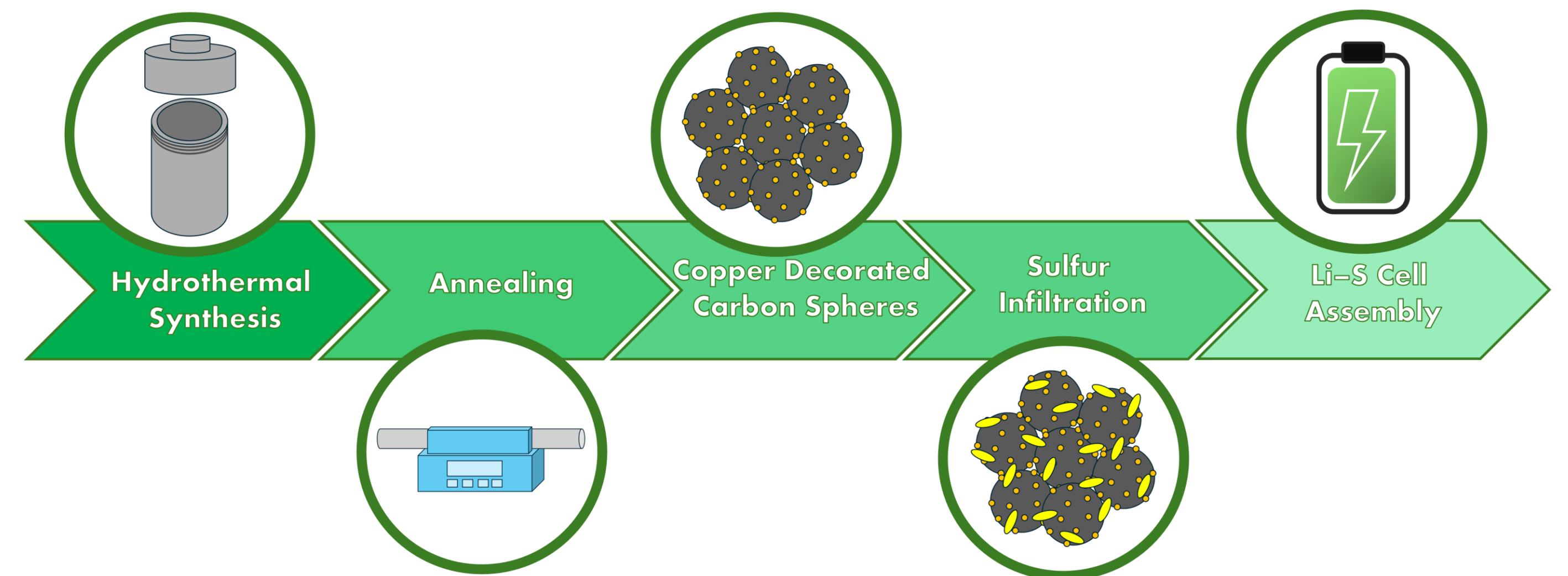
SEM and STEM-EDX imaging show **CuCS** are composed of carbon micro-spheres with copper nanoparticles embedded on the surface. **CS** sample is composed of carbon nano-spheres

XRD of **CuCS** shows three distinct peaks corresponding to the crystallographic planes of cubic copper. **Raman** scattering suggests an amorphous, disordered carbon structure.

XPS reveals primarily SP² Carbon, as well as some oxygen groups. Cu 2P peaks indicate the formation of a native copper oxide layer.

Operando WAXS

SYNTHESIS



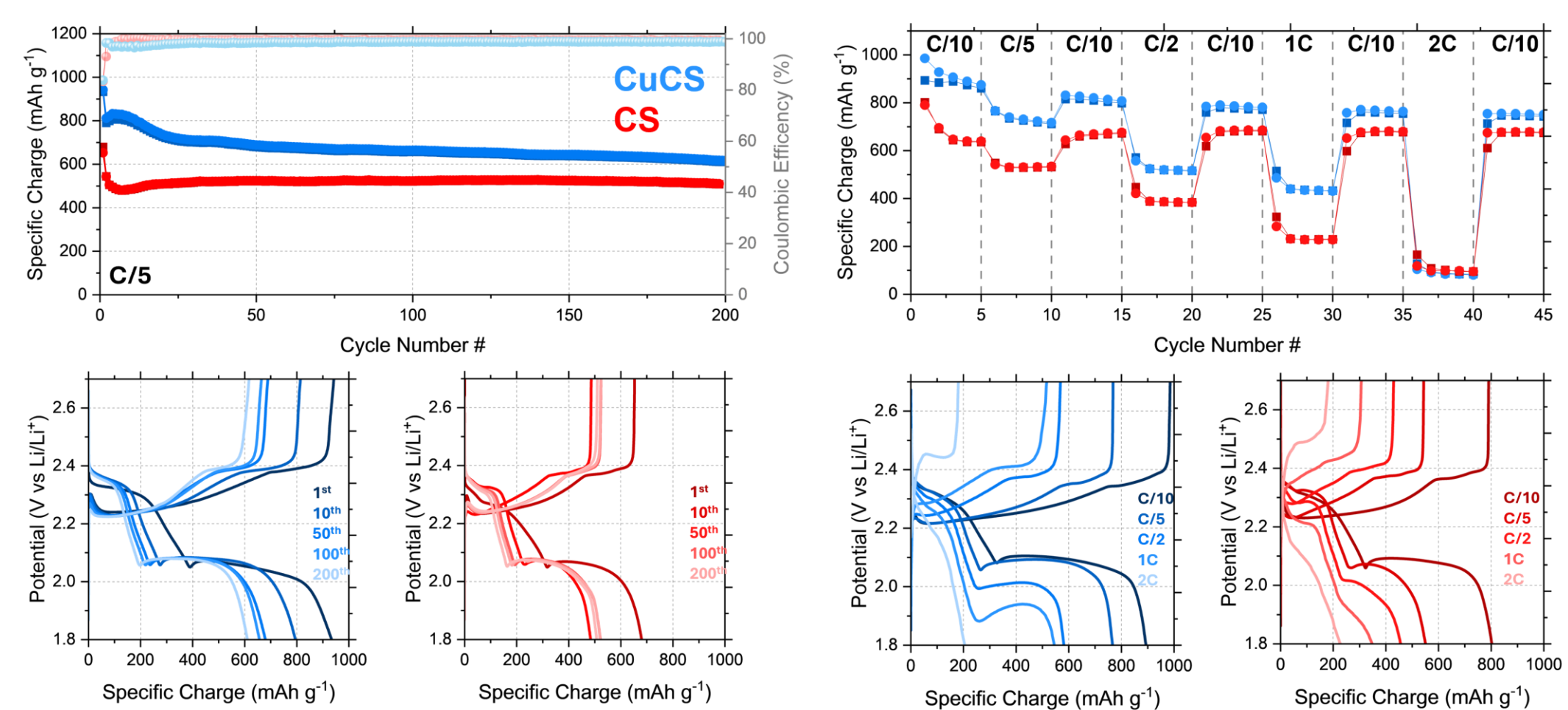
Sugars (e.g. **glucose**, sucrose, fructose) offer an **inexpensive, renewable, and safe** source of carbon that can be converted into **novel functional materials**. This puts them in a unique position to replace petroleum-derived products, a vital step in the transition to a renewables-based economy.

The incorporation of copper nanoparticles should aid in **suppressing the polysulfide shuttle effect** by combining the physical confinement properties of porous carbon spheres with the chemical adsorption capabilities of copper. Moreover, copper is a promising candidate as an **electrocatalyst material** due to its relatively low cost, high electrical conductivity, catalytic availability, and reactivity with sulfur species

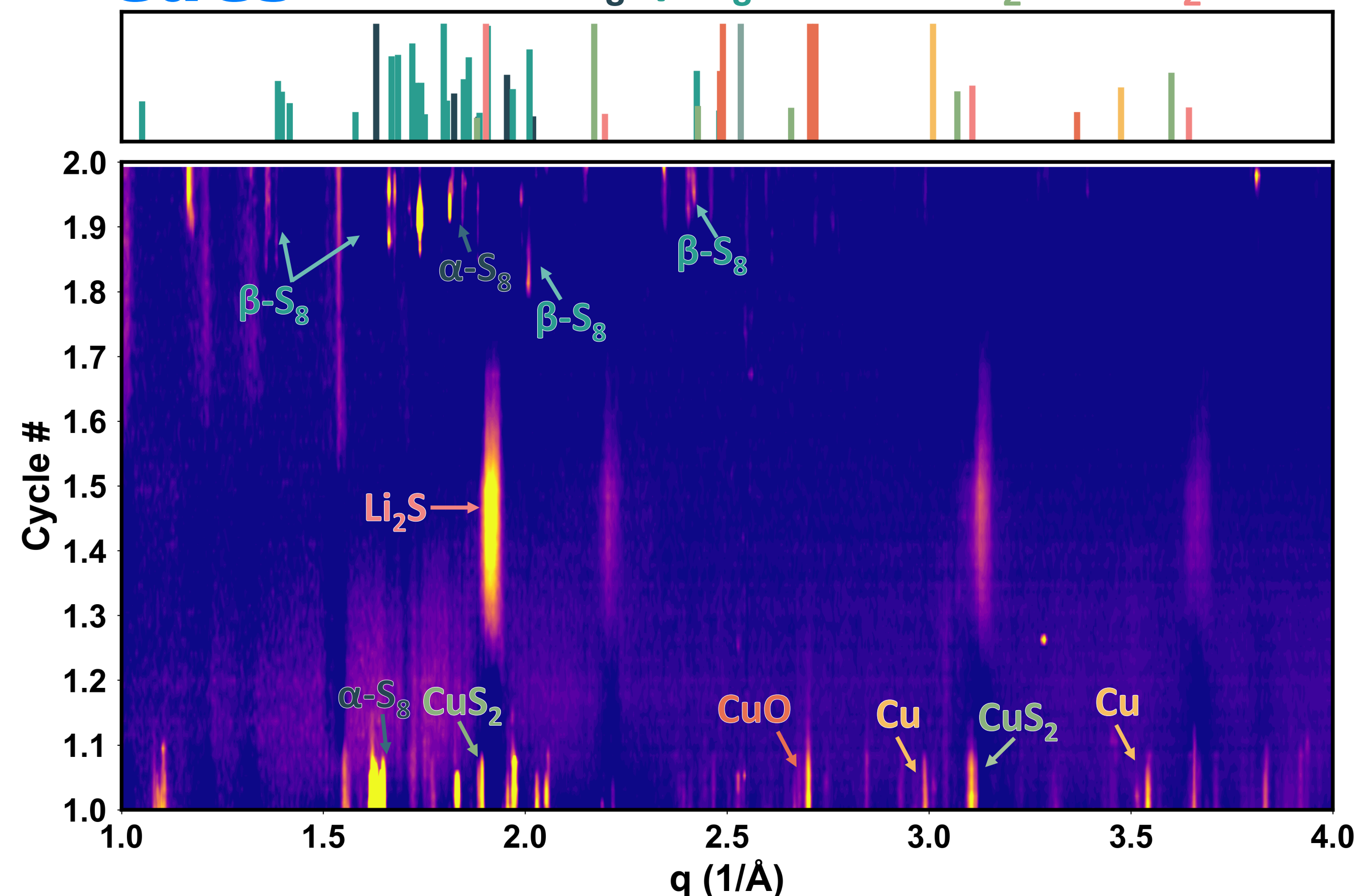
ELECTROCHEMISTRY

CuCS shows a consistently higher specific charge under a constant current of C/5. With an initial capacity of **933 mAh g⁻¹** and **611 mAh g⁻¹** after 200 cycles. **CS** had an initial capacity of **679 mAh g⁻¹** and **508 mAh g⁻¹** after 200 cycles

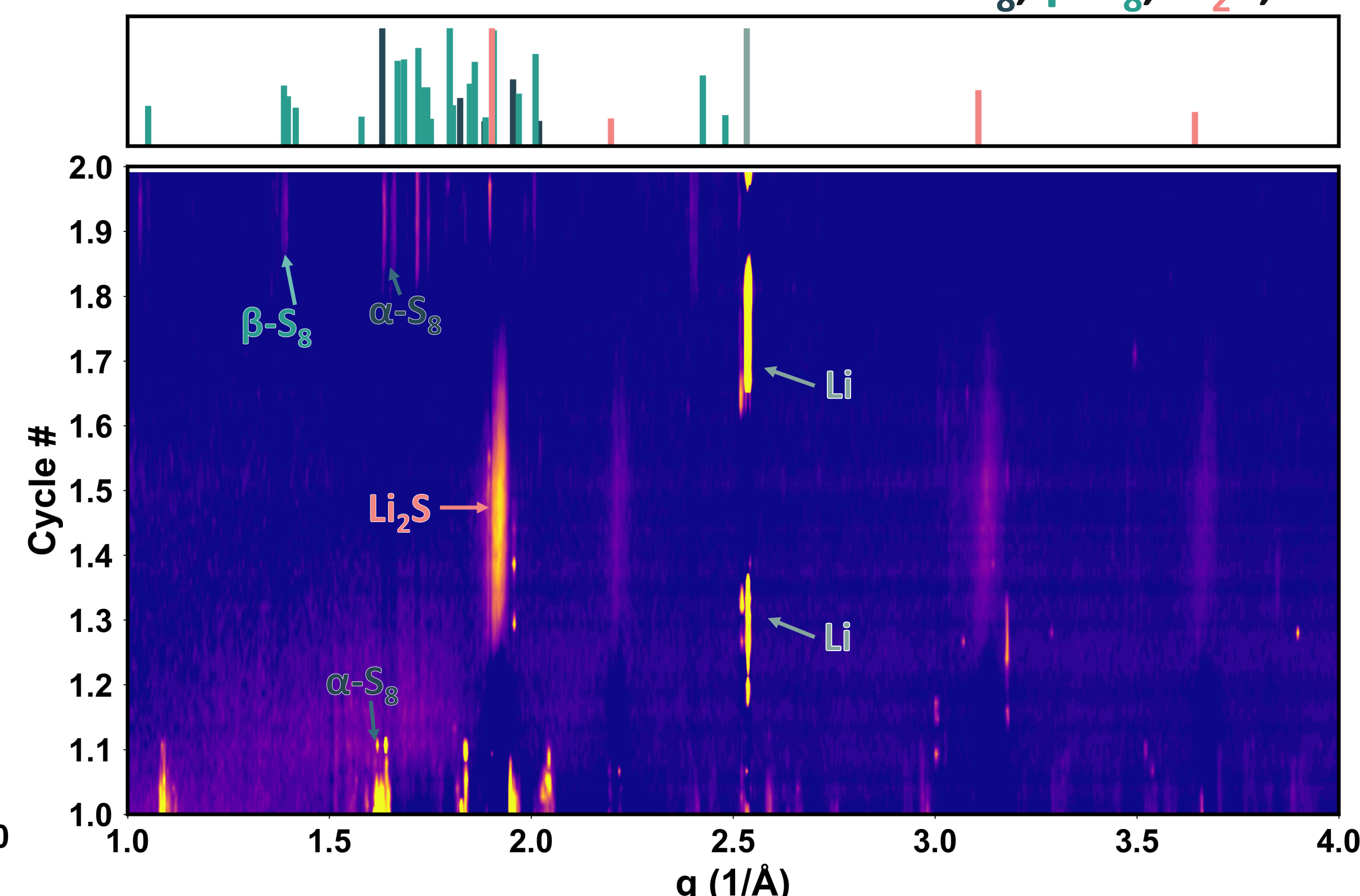
CuCS also shows a significant improvement in rate performance.



CuCS α -S₈, β -S₈, CuO, CuS₂, Cu, Li₂S, Li



CS α -S₈, β -S₈, Li₂S, Li



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CONCLUSIONS

- A novel synthesis technique was developed for the production of copper nanoparticle embedded carbon microspheres.
- The addition of copper nanoparticles to the carbon spheres resulted in a significant increase in specific capacity and capacity retention.
- The mechanism was investigated via synchrotron WAXS, where Cu-CS showed peaks corresponding to CuO and CuS₂. The allotropes and orientation of sulfur after precipitation were seen to shift dependent on the carbon host used.

References

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