

Tailoring the Electrochemical Activity of Magnesium Chromium Oxide Towards Mg Batteries Through Control of Size and Crystal Structure

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MgCr₂O₄ spinel has been predicted to be a promising Mg²⁺ intercalation cathode material for Mg batteries, due to its 3D network of Mg diffusion channels (Figure 1a), and the predicted high electrochemical potential (~3.5 V) of Cr³⁺/Cr⁴⁺ vs. Mg/Mg²⁺.¹ <5 nm MgCr₂O₄ was synthesised via two different methods to produce a regular cubic structure and a highly-defective structure (Figure 1b). The cubic nanocrystals only displayed surface reactivity, whereas the highly-defective nanocrystals achieved reversible deintercalation of Mg from the bulk phase. This was evidenced by post-mortem powder X-ray Diffraction (XRD) and both soft and hard X-ray Absorption Spectroscopy (XAS) analyses. As such, this study represents a breakthrough in the understanding and design of Cr-based spinel cathode materials for Mg-based energy storage.

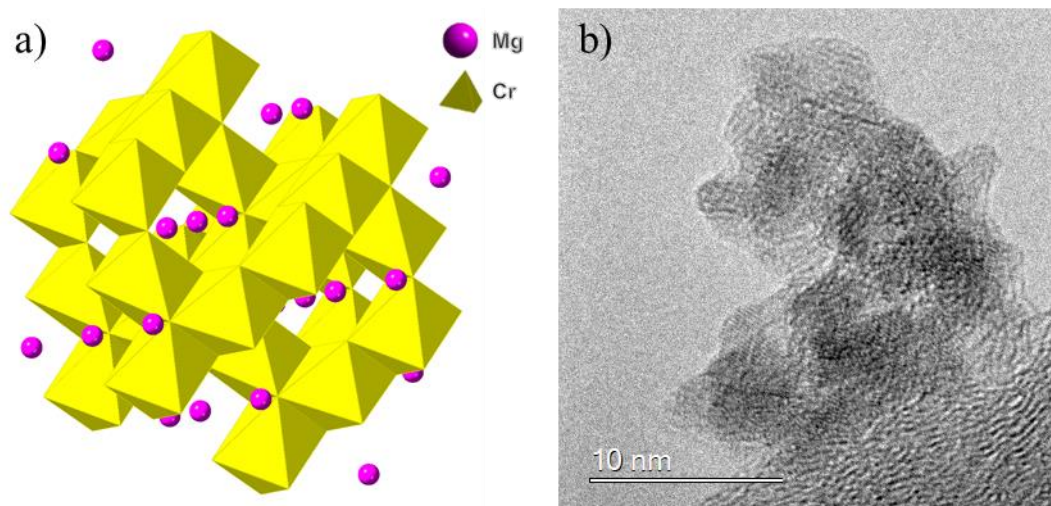


Figure 1: a) The MgCr₂O₄ structure, highlighting the 3D network of Mg diffusion channels. b) A TEM image of a representative highly-defective MgCr₂O₄ particle cluster.

References

- [1] Liu, M; Rong, Z; Malik, R; Canepa, P; Jain, A; Ceder, G; Persson, K A; Liu, M. Spinel compounds as multivalent battery cathodes: a systematic evaluation based on ab initio calculations, *Energy Environ. Sci.* **2015**, 8, 964–974.