
Contribution ID: **134** Type: **Poster**

# Exploring the lithium intercalation mechanism and critical role of structural water in layered H2V3O8 high-capacity cathode material for lithium-ion batteries

*Tuesday 21 March 2023 16:00 (2 hours)*

H2V3O8 (HVO) is a promising high-capacity cathode material for lithium-ion batteries (LIB). It allows reversible two-electron transfer during electrochemical lithium cycling processes, yielding a very attractive theoretical capacity of 378 mAh g−1. Aimed at providing insights into the lithium storage behavior of HVO, we employed a combination of high-resolution synchrotron X-ray and neutron diffraction to accurately describe the crystal structures of both pristine and lithiated H2V3O8. The role of water in network stabilization was examined using density functional theory (DFT) calculations. Furthermore, magic-angle spinning (MAS) NMR spectroscopy allowed to follow the influence of structural water on the intercalated lithium in the crystal host. and related . The hydrogen bonds mitigate the volume expansion/contraction of vanadium layers during Li intercalation/deintercalation, resulting in improved long-term structural stability, explaining the excellent performance in rate capability and cycle life reported for HVO in LIBs. This study suggests that many hydrated materials can be good candidates for electrode materials in not only implemented Li technology but also emerging rechargeable metal-ion batteries.

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**Session Classification:** Poster session TUESDAY

**Track Classification:** Chemistry of Materials (Structure and Spectroscopy)