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Structural evolution of layered H2V3O8 high-capacity lithium storing cathode

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V-based oxides are attracting much interest as promising next-generation electrodes due to the vast resources in the Earth's crust, their unique open structures for fast diffusion with outstanding electrochemical properties and various oxidation redox couples. A recent review has debated if they "will become the future choice for ion-metal batteries".[1] H2V3O8 allows reversible two-electron transfer during electrochemical lithium cycling, yielding a high capacity of 378 mAh g–1. Aimed at providing insights into the lithium storage mechanism, we employed high-resolution synchrotron X-ray and neutron diffraction to accurately describe the crystal structures of both pristine and lithiated H2V3O8.[2] Easy hydrogen-bonding switch of structural water upon lithium intercalation not only allows better accommodation of intercalated lithium ions but also enhances Li-ion mobility in the crystal host, as evidenced by MAS-NMR spectroscopy. The hydrogen bonds mitigate the volume change of vanadium layers during Li de/intercalation, resulting in improved long-term structural stability. This study suggests that other hydrated oxides may be good candidates as electrode materials not only in implemented Li technology but also emerging rechargeable post-lithium metal-ion batteries.

1 D. Zhao, et al. ChemSusChem, 15, e202200479 (2022)
2 A. Kuhn, J. C. Pérez-Flores, J. Prado-Gonjal, E. Morán, M. Hoelzel, V. Díez-Gómez, I. Sobrados, J. Sanz, F. García-Alvarado, Chem. Mater., 34, 694-705 (2022)

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