

Article title: Preparation, Structure Study and Electrochemistry of Layered H₂V₃O₈ Materials: High Capacity Lithium-Ion Battery Cathode

Authors: Sudeep sarkar; Arghya Bhowmik; Jaysree Pan; Mridula Dixit; Sagar Mitra

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Abstract

The present study explores H₂V₃O₈ as high capacity cathode material for lithium-ion batteries (LIB's). Despite having high discharge capacity, H₂V₃O₈ material suffers from poor electrochemical stability for prolonged cycle life. Ultra-long H₂V₃O₈ nanobelts with ordered crystallographic patterns are synthesized *via* a hydrothermal process to mitigate this problem. The growth of the crystal is facile along [001] direction, and the most common surface is (001) as suggested by Wulff construction study. Electrochemical performance of H₂V₃O₈ cathode is tested against Li/Li⁺ at various current rates. At 50 mA g⁻¹ current rate, it delivers a discharge capacity of 308 mAh g⁻¹, whereas, at 3000 mA g⁻¹, an initial discharge capacity of 144 mAh g⁻¹ is observed and stabilized at 100 mAh g⁻¹ till 500 cycles. Further, the density functional theory (DFT) based simulations study of both the pristine and lithiated phase of H₂V₃O₈ cathode materials is undertaken. DFT study reveals the presence of hydrogen as hydroxyl unit in the framework of the host. In correlation, the magnetic property of vanadium atoms is examined in detail with through partial density of states (PDOS) calculation during three stage lithiation processes and evaluating various potential steps involved in lithium insertion.

