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

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Web link: http://www.sciencedirect.com/science/article/pii/S0378775316310837

Source/Publisher: The International Journal on the Science and Technology of Electrochemical Energy Systems

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−1current 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.