
Seminar

(De)lithiation Mechanism of Vanadium Sulfide, a Promising Conversion Electrode Material for Rechargeable Lithium Ion Batteries

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The low theoretical capacities of the conventional LiCoO_2 cathode materials ($120\text{-}150 \text{ mAh g}^{-1}$) and graphite anodes (372 mAh g^{-1}) used in rechargeable Li ion batteries fuels an intense search for alternative electrode materials capable of higher electrical storage capacities. One way of achieving a larger specific capacity is to explore materials that are capable of undergoing a wider change in oxidation states thereby allowing for the accommodation of more than one Li ion per transition metal ion leading to higher capacities. We have found that VS_4 , which is found as the mineral patronite, also described as $\text{V}^{4+}(\text{S}^{2-})_2$, has enormous potential as an electrode material in combination with graphite oxide, with preliminary electrochemical data indicating a remarkably high charge capacity close to 900 mAh/g . This material crystallizes in the monoclinic symmetry and is comprised of uncommon eight-coordinate V^{4+} ions coordinated to S^{2-} dimers which are linked together as linear chains with alternating bonding (2.8 \AA) and non-bonding contacts (3.1 \AA) between the vanadium centers. The products of discharge/charge are nano-sized and therefore difficult to characterize by conventional crystallographic methods. Pair Distribution Function analysis combined with Solid State NMR and XANES indicate that the VS_4 is partially reversible and undergoes a unique internal redox process during discharge in which electron transfer from the V to S leads to the breaking of sulfur dimers and formation of a tetrahedral intermediate.

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4:00 PM (Tea/Coffee at 3:45 PM)

Seminar Hall, TCIS