Bachelor or master thesis

Doped V_2O_5 as Mg^{2+}-insertion electrode for magnesium rechargeable batteries

Starting date June 2016 and later

Vanadium pentoxide (V_2O_5) has layered structure which can accommodate various guest species such as Li^+, K^+, Na^+, as well as Mg^{2+}. It has high theoretical energy density of 1200 Wh/kg based on 4 mol of Mg^{2+} intercalation into V_2O_5. However, up to now only limited Mg^{2+} ion capacities have been achieved for this kind of cathode material. One of the major problems associated with the electrochemical chemical performance of V_2O_5 is the strong polarization of the small divalent Mg^{2+} (0.72 Å) which retards the diffusion of Mg^{2+} ions. First principle calculations have shown that the hopping barrier of Mg^{2+} ions in V_2O_5 is 1.26 eV, which is much higher than that of Li^+ ions (0.35 eV).

In this work two strategies are proposed to improve the intercalation of Mg^{2+} in the V_2O_5 cathode: (1) to prepare dedicated nano sized V_2O_5 materials. Due to short diffusion length for Mg^{2+} ions, the nanosized materials can alleviate (at least, partially) the intrinsic limitations associated with slow solid-state diffusion of Mg^{2+} ions. (2) to synthesize cation doped V_2O_5 materials. The doping cations can modify the crystal and electronic structure of V_2O_5, and, therefore, can have a strong impact on the ionic or electronic conductivities. Since the enhancement of lithium transport in V_2O_5 upon doping has already previously been reported, this approach looks very promising for magnesium-based systems.

The nanostructured V_2O_5 as well as Cu- and Co-doped V_2O_5 will be prepared by hydrothermal method. The characterization of the materials obtained will be performed by powder X-ray diffraction, scanning electron microscopy (combined with EDX element mapping) and electrochemical methods (cyclic voltammetry, galvanostatic cycling) in the half-cells.

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