Overcoming the current limitations of Li-ion batteries using alternative synthesis routes for conversion electrode materials

M.A. Muñoz-Márquez^{1,*}, B. Acebedo¹, C. Bernuy-López¹, P. Bline^{1,2}, E. Castillo-Martínez¹, M. Galcerán¹, E. Gonzalo¹, E. Lefebvre^{1,2}, M. Casas-Cabanas¹

¹ CIC energiGUNE, Albert Einstein 48, 01510 – Miñano, Spain.

² ENSICAEN, FR3095 Caen, France.

^{*}E-mail: mamunoz@cicenergigune.com

The electrodes used in commercial Li-ion batteries are intercalation materials such as LiFePO₄, which act as a matrix where Li ions are inserted and deinserted. In this case, the capacity depends on the available number of sites for Li accommodation: typically, 0.5-1.0 electrons per formula unit leading to theoretical specific capacities of 170 mAhg⁻¹.

For Li-ion technology to consolidate in the continuously miniaturizing portable electronics market and take over the electric vehicle a qualitative increase in capacity is needed. Electrode materials based in conversion electrochemistry are a promising choice for the capacity enhancement [1], in fact, transition metal-based conversion materials allow using all possible oxidation states in which more than one electron transfer occurs per transition metal ions with theoretical specific capacities as high as 1500 mAhg⁻¹.

Ever since the reversible conversion reaction was reported for Li-ion batteries [2], there is a growing interest in the scientific community on this family of materials. Up to date transition metal oxides, hydrides, sulphides, nitrides and fluorides [3-6] have been considered as suitable electrodes for Li-ion conversion batteries.

Based on the previous studies on conversion materials we have proposed new materials and alternative optimization strategies that intend to address the main problems of conversion materials namely voltage hysteresis, cycle life and reversibility. The investigation of the electrochemical properties using cyclic voltammetry was complemented with the structural characterization by means of X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Additionally, the surface composition was studied using X-ray photoelectron spectroscopy (XPS). Therefore we can ensure that a complete picture of the driving mechanisms of the cycling process is obtained.

Significant improvements in the cycle life will be presented. Moreover, the new sought synthesis routes have resulted in active materials with greatly enhanced specific capacities.

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