



Master or Bachelor Thesis

“Synthesis of novel anodic compositions based on partial and total substitution of lithium with a divalent metal in $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ NASICON-type material”

Starting date: April 2017 or later

Exploring and designing novel structures which enables enhanced capacity and at the same time excellent rate capability is a challenging goal for the development of batteries and supercapacitors. The NASICON-type $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ (LVP) material is very promising as high power capability cathode material in the potential range 3 - 4.3 V vs. Li/Li^+ [1]. However, due to its amphoteric nature LVP can also host additional lithium ions and can therefore be used as anode in the potential range 3 – 0 V vs. Li/Li^+ [2]. When used as anode LVP display the high capacity of 250 mAh g^{-1} at 1C. However, in this potential range its rate capability is inferior to the one obtained between 3 – 4.3 V vs. Li/Li^+ . Strategies to facilitate the ion diffusion and insertion in these structures are therefore highly desirable.

The purpose of this work is to partially substitute Li^+ with the divalent M^{++} ($\text{M}=\text{Ca}$, Mg and Co) in order to create more vacancies in the structure and help to facilitate the Li^+ insertion/deinsertion in the material. This concept idea was inspired by the paper of Z. Wei et al [3] who in a similar way explored the NASICON-type material $\text{Ca}_{0.5}\text{Ti}_2(\text{PO}_4)_3$ for Na-ion batteries. In this work the substitution of Na^+ with the divalent Ca^{++} was of extreme benefit to improve the rate capability and capacity.

The work will involve the synthesis and characterization of various compositions based on partial or total substitution of lithium with the divalent M (e.g. $\text{M}_{0.5}\text{Li}_2\text{V}_2(\text{PO}_4)_3$, $\text{MLiV}_2(\text{PO}_4)_3$ etc.).

Moreover, electrochemical characterization including cyclic voltammetry, galvanostatic charge/discharge cycles and electrochemical impedance spectroscopy will be also conducted.

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Literature

- [1] M. Secchiaroli G. Giuli, B. Fuchs, R. Marassi, M. Wohlfahrt-Mehrens and S. Dsoke, „High rate capability $\text{Li}_3\text{V}_{2-x}\text{Ni}_x(\text{PO}_4)_3/\text{C}$ ($x=0, 0.05$ and 0.1) cathodes for Li-ion asymmetric supercapacitors”, J. Mater. Chem A, 3 (2015) 11807-11816
- [2] X. Zhang, R.-S. Kühnel, M. Schroeder and A. Balducci, „Revisiting $\text{Li}_3\text{V}_2(\text{PO}_4)_3$ as an anode – an outstanding negative electrode for high power energy storage devices“, J. Mater. Chem A, 2 (2014) 17906-1713
- [3] Z. Wei, X. Meng, Y. Yao, Q. Liu, C. Wang, Y. Wei, F. Du and G. Chen, „Exploration of $\text{Ca}_{0.5}\text{Ti}_2(\text{PO}_4)_3$ @carbon Nanocomposite as the High-Rate Negative Electrode for Na-Ion Batteries“, Applied Materials and Interfaces 8 (2016) 35336-35341