



PhD thesis proposal (UMICORE / IMN) – October 2018

Title: Characterization of surface reactivity of Ni-rich positive material for Li-ion batteries

Lithium-ion battery technology is the main contributor to the electrification of vehicles. It relies on layered oxide materials of general composition $\text{LiNi}_{1-x-y}\text{Mn}_x\text{Co}_y\text{O}_2$ (NMC) as positive active material. Improvements in terms of energy densities, cycle life and costs are still expected to allow a significant market penetration of electric vehicles. Today, the market is heading towards high-nickel NMC (80% or more nickel content, achieving 200 mAh/g reversible capacity) because they provide higher energy densities. Cycle stability of Li-ion batteries is related to intricate effects of the stability of the interfaces between the active materials and the liquid electrolyte. It has been largely observed that batteries using high-nickel NMC suffers from severe gassing issues, which drastically reduces the cycle life and causes severe safety concerns.

The main objective of this PhD proposal is to elucidate the origin of gas generation from high-nickel materials via a systematic study. It has been argued that the gas generation originates from the surface collapse of NMC (releasing oxygen), the high reactivity of Ni^{4+} cations towards the carbonate electrolyte or the presence of lithium impurities (Li_2CO_3 , LiOH ...) at the surface of the active materials. The PhD proposal aims at gaining a deeper insight of this issue via a systematic study of several parameters:

This research project will be carried out at the Institut des Matériaux Jean Rouxel (IMN), located in Nantes, which has a strong experience in analytic techniques to study surface and bulk phenomena. The work will be supported by Umicore, leader in the commercialization of layered oxides for battery application.

Starting materials will be provided by Umicore although the research project aims to set up model experiment to emphasize and study specific parameters. The first step of the PhD work will be to obtain a complete analysis of surface properties of such materials. Electron energy-loss spectroscopy (EELS), X-ray photoelectron spectroscopy (XPS), high-resolution transmission electron (HR-TEM) and nuclear magnetic resonance (NMR) will allow characterizing the crystalline structure and the chemical composition of the surface of pristine materials. In that regards, the student will benefit from the new equipment recently acquired by IMN. Quantification of lithium impurities will be performed by combining EELS and solid state NMR. The materials will be then tested in pouch cells of 600 mAh. Measurement of volume expansion will give insights on the gassing of the system. This study will possibly be completed by on line chemical characterization of gas at NIMBE/LYONS laboratory in Saclay. Post-mortem analysis will complement the study.

Applicant profile: you have obtained a Master degree (M2 or equivalent) in Materials science (preferably), Physics, Chemical-Physics or equivalent. You have a good knowledge of characterization techniques such those given above. You are meticulous, rigorous, and not afraid of data processing. You have a strong interest in understanding physical and chemical phenomena. You are able to fit easily in a team and produce regular reports to academic or non academic partners.

Contact: CV + application letter + last 2 year marks to:

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