icmcb
institut de chimie de la matière condensée de bordeaux

**PhD position (2016-2019)**

# Structure and Dynamics in Layered Oxides and Phosphates Materials for Na-ion batteries: A Combined NMR and DFT Calculations Approach

This PhD project, will allow establishing a new collaborative effort between two internationally recognized research teams, working in the area of alternative energy materials, and builds on their complementary expertise to tackle the merging topic of **sodium-ion batteries**. It will strongly reinforce the FFCR (Fonds France-Canada pour la Recherche) project on "Structure and Dynamics of Sodium Ion Cathode Materials: New Strategies for Electric Vehicle Energy Storage" just accepted between D. Carlier at ICMCB (**Institut de Chimie de la Matière Condensée de Bordeaux**) and G. Goward (**McMaster University, Hamilton, Ontario, Canada).**

Lithium ion batteries have achieved success in the portable electronics market and are currently the leading technology for vehicle electrification in the automotive industry. However, supply-and-demand pressures on the market, paired with the escalating use of Li, are expected to increase the cost of Li materials substantially. As a result, sodium ion ($Na^+$) batteries have risen to the forefront as a viable alternative to Li owing to the enormous and inexpensive global supply of sodium and theoretically comparable electrochemical performance. Furthermore, limited transition metal resources required for electrode materials has perpetrated the desire to incorporate reasonably abundant elements such as Fe or Mn into Na ion battery cathodes. Relative to Li, the field cathode material development for Na ion batteries is still in its infancy, and despite similarities between Li and Na electrochemistries, there is considerable work to be done to aid in the realization of appropriate Na materials in order for Na ion batteries to compete in the commercial market.

Layered oxide materials have received attention for both Li and Na as they offer excellent electrochemical performance for both alkali ion analogs. Moreover, the continued desire to match the success of the celebrated Li olivine ($LiFePO_4$) phase has resulted in significant efforts to produce iron-containing Na phosphate derived materials whose performance rivals that of the oxides. Attractive candidates such as the layered fluorophosphate or NASICON structures have shown promise due to their excellent thermal and electrochemical stability during charge/discharge processes coupled with encouraging electrochemical results. There is a need to look closely at the mobility and chemical changes that the cathode material undergoes as a function of the charge/discharge process in order to gain insight into unique properties that might aid in performance. In this PhD project, we plan to study classes of materials such as the **layered oxides $Na_xMO_2$ (M = 3d transition metal) and phosphates as $NaFePO_4F$, and $Na_3Fe_2(PO_4)_3$** chosen either their robust structures and low-cost, low-toxicity transition metals (iron), or identified as ideal cathode candidates for further investigation.

The proposed combination of experimental and computational studies will build a new collaborative effort between the G. Goward and D. Carlier research teams in the area of next-materials for alternative energy devices. The methodology to be used in our research program will bring together state-of-the-art **Solid state chemistry and electrochemistry, solid-state magnetic resonance spectroscopy (NMR) and electronic structure calculations (based on the Density Functional Theory (DFT))**. These complimentary tools will allow us to fully correlate the structures of the materials with


ICMCB-CNRS – Université de Bordeaux
87, avenue du Dr Albert Schweitzer
33608 Pessac cedex (France)
Tél. : +33 (0)5 40 00 26 50 - Fax : +33 (0)5 40 00 66 34
*http://www.icmcb-bordeaux.cnrs.fr*

their spectroscopic properties, which is the first step toward understanding the function of the cathode within an electrochemical device.

**The PhD candidate should have a background in solid state chemistry and chemical physics. Some periods at Mc Master University will be scheduled but the PhD diploma will be delivered by the Bordeaux University. The MENRT PhD fellowship is already ensured and expected starting date is October 1st 2016.**

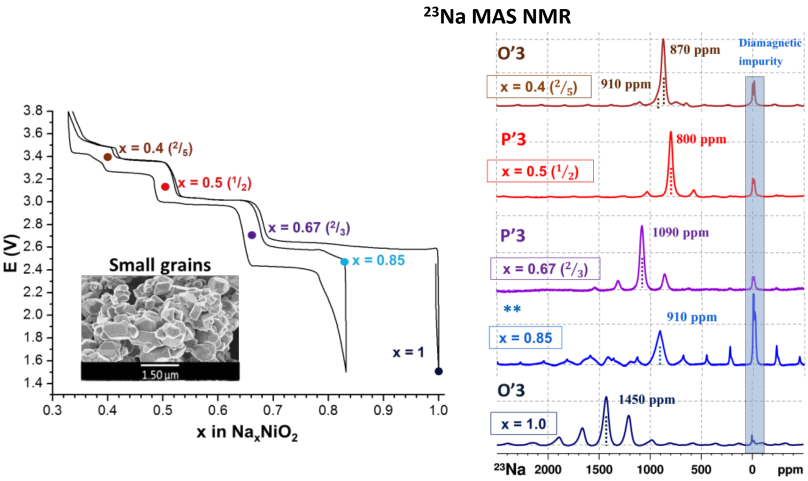


**Figure** : Electrochemical cycling curve of a Na//$NaNiO_2$ battery (C/20) and $^{23}$Na MAS NMR spectra of intermediate selected phases ($\nu_r$ = 30 KHz with $B_0$ = 11.75 T)

Please contact:


**Dany CARLIER-LARREGARAY**

***Maitre de Conférences à l'Université de Bordeaux (HDR)***

***Institut de Chimie de la Matière Condensée de Bordeaux (ICMCB-CNRS)***

Tél. : +33 (0)5 40 00 35 69

Fax : +33 (0)5 40 00 66 34

*E-mail :dany.carlier@icmcb.cnrs.fr*