Laboratoire d'Electrochimie et de Physico-chimie des Matériaux et des Interfaces (UMR 5279)

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Understanding the Lithiation Reaction Mechanisms in Advanced Electrode Materials for Lithium Batteries

Keywords: Solid state chemistry, electrochemistry, Li-ion battery, *operando* characterization

Offer description

Although being the most commonly used negative electrode material, graphite still suffers from limitations especially its poor fast charging ability. This phenomenon can lead to the formation of metallic lithium deposits (so called plating) that can lead to dendrites responsible of internal short circuits.

The spinel $Li_4Ti_5O_{12}$, another negative electrode material, prevents the formation of these dendrites due to its higher operating potential. However, despite a *"power"* ability, this material has a low specific capacity and energy density. Alternative materials need to be developed to tackle the challenge of fast charging ability. $TiNb_2O_7$, a Wadsley-Roth type phase, stands out as an alternative negative material with growing interest, offering high specific capacity and a higher specific energy while maintaining fast-charging capabilities. However, the reaction mechanisms governing the lithium insertion into the crystal structure are still poorly understood.

The objective of this master thesis is to synthetize the materials using solid state chemistry route, as an example via ball milling and characterize it in terms of electrochemical performance. The ultimate goal is to perform *operando* measurements through neutron and/or synchrotron X-ray diffraction to determine the lithiation mechanisms.

The master thesis will be located in Grenoble at LEPMI laboratory, if needed additional investigation at Grenoble Large-scale facilities (synchrotron and neutron) will be employed.

Goals

- Synthesis of the material and electrode preparation
- Characterization of the electrochemical performance on half-cells
- Material characterization by diffraction techniques in large-scale instruments and data processing
- Writing elaboration protocols and experimental reports

Student profile: We are looking for a Master student with a background in material science and/or chemistry. Electrochemical interest/experience is an asset.

Duration: 6 months

Location: LEPMI (laboratory on Grenoble Campus, France)

Starting date: February 2025

To apply to this master thesis please send your CV and motivation letter to Benjamin Mercier-Guyon (benjamin.mercier-guyon@grenoble-inp.fr) and Sergio F. Mayer (sergio-federico.mayer@grenoble-inp.fr)