2021-2022

Master thesis proposal

Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie

Campus Pierre et Marie Curie
Tower 23 - 4th floor -23-22
Director: A. Marco Saitta

Title: Role of water in the colossal permittivity of $Rb_2Ti_2O_5 : (H2O)_x$

Keywords: Functional materials, infrared spectroscopy, ionic conduction, supercapacitors

Scientific description: As supercapacitors can very effectively transport charges and endure many more recharging cycles than available batteries, the search for new materials is a hot topic of current research, at the crossing point between materials science and industrial applications.
Recently, we found that $Rb_2Ti_2O_5$ (RTO) and $K_2Ti_2O_5$ (KTO) show a colossal permittivity that is due to ionic species coming from water incorporation. Placing the materials between two electrodes gives rise to a giant charge accumulation at the anode contact, which deeply affects the intrinsic conductivity. Upon heating from room temperature, the conductivity drops by several orders of magnitude. Moreover, after charging under peculiar temperature conditions a spontaneous current persists for several hours even after the voltage is released. Although the detailed mechanism behind those puzzling trends is still unknown, we know that it deeply depends on the water content **x**. In particular, fully dehydrated samples do not show any of the aforementioned phenomena. Water incorporation therefore modifies the structural and transport properties of the pristine materials.
This internship aims at using several complementary techniques (infrared spectroscopy, electrical measurements and first-principle simulations) to understand the fate of water within RTO and KTO, the equilibrium and transport behavior of the released species OH^- and H^+ upon dissociation, and the possible onset of new charged species from chemical reactions in the materials.
The internship relies on previous work that has been done along two PhD theses and will be conducted in a collaborative, multi-disciplinary environment. The main experiments will be performed at the infrared beamline at the synchrotron SOLEIL under the direction of Paola Giura and simulations run at the INSP (supervised by Fabio Finocchi). Complementary electric measurements will be carried out in collaboration with ESPCI and a Master thesis proposal is also submitted on these measurements (supervised by Brigitte Leridon or Stéphane Holé). The Master student can thus practice several state-of-the-art techniques with an evident benefit for her/his know-how.

Techniques/methods in use: Infrared spectroscopy (main) and DFT calculations.

Applicant skills: Good background in quantum and condensed matter physics, curiosity for experimental investigations, basics of computational methods.

Industrial partnership: Y/N : NO

Internship supervisor(s) : Paola GIURA, paola.giura@sorbonne-universite.fr, tel: +33 1 44275219

Internship location: Institut de Minéralogie de Physique des Matériaux et de Cosmochimie (IMPMC) , Tour 23, 4th floor, place Jussieu.

Possibility for a Doctoral thesis: Y/N (specify if already financed) YES. Ecoles doctorales ED397, ED564 (ED PIF), ANR founding.