

PhD topic: “Multilayered antiferroelectric supercapacitors for green and efficient energy storage: fundamental study for real-life applications”

Doctoral School: « Interfaces » / **Topic:** Solid-state Physics

Lab: Structures, Properties and Modelling of Solids (SPMS)

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Keywords: ferroelectrics, material synthesis, energy storage

Topics: solid-state physics, ferroelectrics, material synthesis through chemical and physical deposition techniques, material characterisation: x-ray diffraction, electronic microscopy, atomic force microscopy, electrical measurements, spectroscopy...

Supervision: This thesis work will be co-supervised by Cosme Milesi-Brault, maître de conférences (expertise on synthesis and spectroscopy of ferroelectrics) and Prof. Pierre-Eymeric Janolin (expertise on structural and electrical properties of ferroics).

Quick summary of the thesis project:

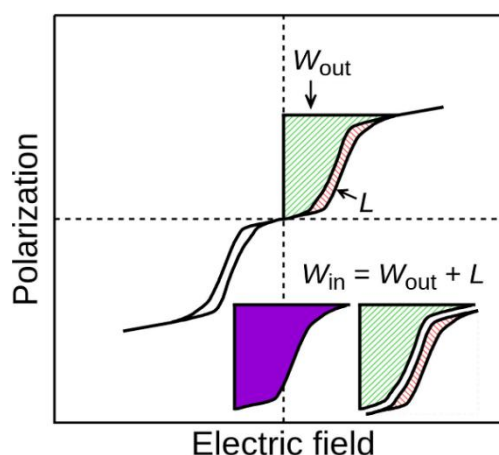
Antiferroelectrics are dielectric materials composed of an antipolar array of dipoles, which display no macroscopic polarisation. They can be switched to a polar ferroelectric phase by application of an electric field: this field-induced phase transition is called switching, which induces a so-called “double hysteresis loop” in its polarisation vs electric field curve. The shape of this double hysteresis loop allows for efficient storage of electrical energy and a very fast discharge, useful for high-power applications [1, 2].

In particular, the development of sustainable alternatives to traditional lead-based ferroelectrics and antiferroelectrics is a crucial step towards creating environmentally friendly energy storage solutions.

On a more fundamental side, layering antiferroelectric and ferroelectric materials could also induce extremely rich topological physics, such as ferroelectric skyrmions [3, 4], which could be further energy storage properties of multilayers [5, 6, 7], but also in other applications (e.g. extremely low-power computing). Investigating how such antiferro/ferroelectric multilayers behave under an electric field (including the underlying mechanisms of electric field-induced phase transitions) is also a very important topic in the ferroic community.

This PhD research project will focus on the synthesis and characterization of novel materials that can replace toxic lead-based compounds in energy storage devices, such as supercapacitors.

Materials of interest are lead-free inorganic perovskites such as BiFeO_3 , NaNbO_3 , AgNbO_3 , $(\text{Nb}_{0.5}\text{Bi}_{0.5})\text{TiO}_3$... which are (anti)ferroelectric materials.



Principle of energy storage in antiferroelectric materials. W_{in} , W_{out} and L respectively indicate the energy density needed to charge the antiferroelectric capacitor, the recoverable energy density and losses. Adapted from Ref. [5].

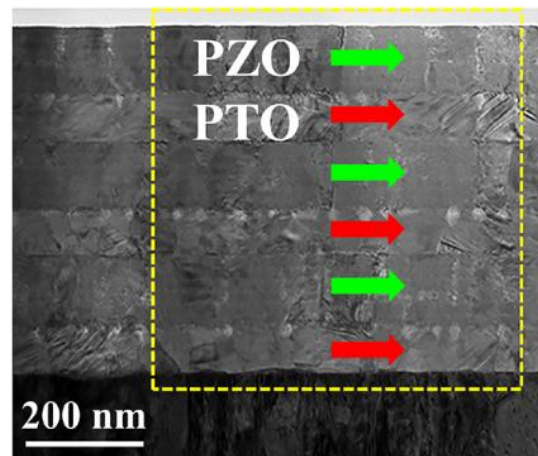
During this PhD, the candidate will:

- Design and synthesise eco-friendly alternatives to standard lead-based (anti)ferroelectrics in the shape of multilayers
- Analyse in-depth the electrical, structural, and chemical properties of these multilayers
- Investigate the suitability of these materials for energy storage devices, particularly supercapacitors, and optimise their performance for enhanced energy density and power density.
- Study *in-situ* (anti)ferroelectric multilayers under the influence of electric fields and temperature change to elucidate their underlying mechanisms of their phase transitions

The first step of this PhD project is to **synthesise lead-free antiferroelectric multilayers** [7] by chemical solution deposition (CSD) and pulsed laser deposition (PLD) and to **optimise their density of storable energy**. The second step of this project is to **shed light on the electric-field induced switching mechanisms of these multilayers** to further improve our knowledge of these materials.

Main experimental techniques:

Chemical solution deposition (CSD) and pulsed laser deposition (PLD) for depositing multilayer thin film materials; x-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM), atomic force microscopy (AFM) for (micro)structural characterisation; x-ray photoelectron spectroscopy (XPS), electron diffraction spectroscopy (EDS) for chemical analysis; electrical measurements (polarisation, capacitance, permittivity).



SEM cross-section image of a multilayer capacitor made by CSD. Adapted from [7].

Bibliography:

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