Magnetic and Multiferroic properties of mixed-anion cuprates tuned by chemical and physical pressures

3-year PhD position
(Oct. 2020 – Sept. 2023)

Supervisor

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A full-time PhD position is available in the department of Inorganic Theoretical Chemistry (CTI) at the Institute of Chemical Sciences of Rennes (ISCR, University of Rennes 1) for a talented and ambitious student. The position is fully funded by the French Research National Agency (ANR).

Magnetoelectric (ME) multiferroics (MF), which combine electric and magnetic dipole orders, are multifunctional materials with a high potential in new technologies. It can be used to reduce computer memory energy consumption, to improve magnetic field sensors or in spintronic applications.[1,2] Two classes have been defined based on the mechanism promoting the spontaneous polar order.[1,2] **Type I ME-MF**, known as proper ferroelectrics, are based on displacive mechanism (lone-pair, geometric and charge ordering), while **type II ME-MF**, also named spin-driven ferroelectrics (SDF), are improper ferroelectrics in the sense that the polar state is driven by a magnetic transition. Unfortunately, **too few ME crystals are known to date**, and even less could lead to industrial applications. Indeed, they usually give a small response (electric polarization, P_S) and need low functioning temperature to exhibit the desired ME-MF properties. Two main routes to overcome these problems have been considered in the past: (1) the elaboration of composite materials and (2) the search of new crystals exhibiting improved ME-MF properties.

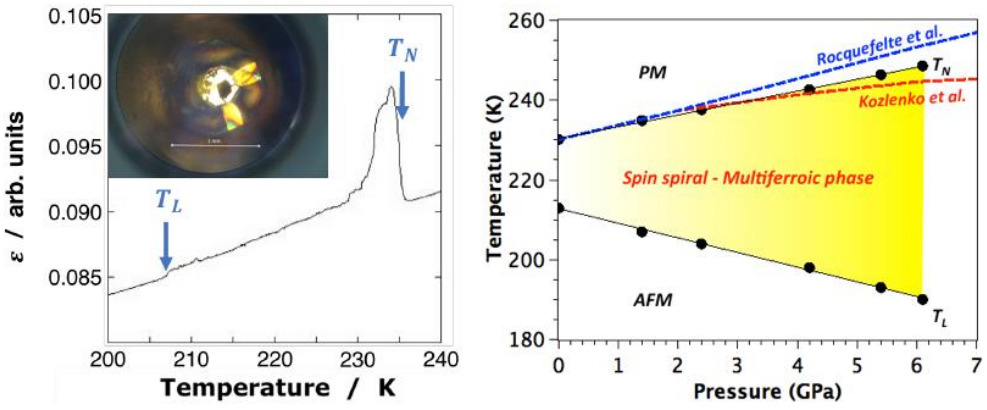

Figure. Left: Dielectric constant (capacitance) measurement on a single crystal of CuO under a pressure of 1.4 GPa. At T_N a large jump of the signal occurs. At T_L a much smaller but still clearly visible anomaly is seen. The inset shows the sample of CuO pressurized in the diamond anvil cell for dielectric constant measurements seen through the diamonds. Right: Schematic representation of our recent measurements of T_N and T_L (black dots) under high-pressure.

We aim at the investigation of a series of compounds (known to be ME-MF or not) having the following specifications: (1) large magnetic exchange couplings in order to reach high temperature functioning and (2) magnetic frustrations to have a strong ME-MF coupling mechanism based on exchange-striction and thus large ferroelectric polarization (P_s). Cuprates are ideal candidates for these two reasons and interestingly exhibit both types I and II ME-MFs.[3-6] **The present project combines advanced experimental techniques** (X-ray, neutron and Raman techniques under pressure, magnetometry, dielectric measurements…) and **state-of-the-art calculations** (density functional theory (DFT), multireference wavefunction (WFT) calculations and Monte-Carlo (MC) simulations).

The present PhD thesis is part of an ANR project named HTHPCM which **combines advanced experimental techniques** (X-ray, neutron and Raman techniques under pressure, magnetometry, dielectric measurements…) and **state-of-the-art calculations** (density functional theory (DFT), multireference wavefunction (WFT) calculations and Monte-Carlo (MC) simulations). The main **goal of this project** is the search of high-temperature and high-polarization cuprate multiferroics (HTHPCM), i.e. (1) with a **large ME-MF coupling** and thus large P_S, (2) **operating at room-temperature** (RT), and (3) showing an **electric-field magnetization reversal**. Our focus is cuprate MFs.

The CTI team

The PhD student will work in the Inorganic Theoretical Chemistry (CTI) team, in the Institute of Chemical Sciences of Rennes. The CTI team gathers several theoreticians (14 permanent staff members, 15 students) with complementary skills in theoretical chemistry but also physics, working with a broad set of quantum chemical tools, ranging from high precision *ab initio* wavefunction-based calculations to fast semi-empirical methods. The studied systems in CTI are diverse, including isolated species, bulk materials and surfaces, mainly of high experimental and societal interest. This has led to fruitful joint collaborations with experimentalists from ISCR as well as major national and international groups. The team is also strongly involved in the collective effort made by the French community of theoretical chemists at the national level, in the quest of bridging the gap between state-of the art quantum tools and real-life applications. The CTI team thus provides a stimulating scientific environment, also offering regular team meetings, invited seminars as well as visitors internationally recognized. Local and national computing means are available for the purposes of the scientific projects.

Profile of the candidate

The PhD will be in charge of the DFT calculations to generate all structural models under chemical and physical pressure. He will also estimate the elastic and vibrational properties (phonon calculations) and estimate the electric polarization. In addition, he will do two or three stays of 2 months in the PHELIQS laboratory) to respectively, (1) participate to the elaboration of single crystals, and to do the complete structural characterization, (2) learn how to setup high-pressure experiments and (3) to participate eventually to a high-pressure experimental campaign. ***The selected student will have a solid experience in solid state science and DFT calculations.*** *Refs 7-10 illustrate the theoretical strategy we will use during the PhD.*

Application

The PhD project will start in October 2020. Applications are already open and candidates shall contact both supervisors by e-mail, with a CV and a motivation letter, including clear description of previous Master internship(s).

References:

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