PhD project proposed at the Institut de Physique de Rennes

Department Materials and Light

Title:

Advanced crystallography of photoactive and multiferroic molecular materials under light
Financial support: contrat doctoral ordinaire (CD0) de l'Université de Rennes 1

PhD supervisors: Elzbieta Trzop (Research Engineer) / Eric Collet (Professor)

Scientific project:

Multistable molecular materials can change their electronic state under the effect of temperature, pressure, light or even magnetic or electric fields.[1-7] These systems present changes of magnetic states linked to a spin transition and/or charge transfer around transition metals. Recently, we have been interested in systems for which the change of electronic state is coupled to a change of symmetry [1-7], which makes the materials multi-functional such as (ferro)magnetic, ferroelastic and/or or ferroelectric. The coupling between change of electronic state and change of symmetry then makes it possible to control ferroelectricity by switching the electronic state using a magnetic field or light, to control magnetism by applying an electric field to switch the ferroelectric polarization, or to play on the ferroelastic distortions of the network with the change of symmetry. Crystallographic studies at equilibrium and/or under light irradiation make it possible to study microscopic processes at the crystalline and molecular scale. The experiments are carried out at the IPR or on a synchrotron when a more powerful X-ray source is necessary, as well as for ultrafast measurements.[9] A theoretical model that we have recently developed [8,9] explains the importance of these couplings and various associated phenomena. We are solicited by different groups (Ireland, Spain, USA, Japan, Thailand) [1-7], to carry out advanced crystallographic studies and to explain and model the phenomena observed with our original approach considering electronic, structural and/or symmetric bistabilities.

Project:

This thesis funding aims to develop our own research projects around the advanced crystallography of photoactive and multiferroic molecular materials. Light represents a parameter of choice for controlling ferroelectricity or magnetism. Crystallography is a central technique for observing changes in structure and symmetry, especially lattice distortions. In 2022 we will acquire a new X-ray source and a cryostat to carry out structural studies in the range [30-300 K] where the phenomena are observed. This will allow advanced crystallographic analyses, at equilibrium and under light, to measure order parameters related to changes in electronic states (lengths of bonds) or changes in symmetry. The knowledge of these parameters allows a direct description within the framework of the Landau theory of phase transitions, and the recently developed model [9] will be improved to describe the metastable states observed recently. In addition to structural reorganization, electronic/structural state changes are associated with a change in color, conductivity, polarization or magnetism. We therefore wish to develop new collaborations for the effects induced by magnetic field and for the effects induced by electric field. Finally, for materials where electronic and ferroelectric bistability are coupled, we plan to study the response of these systems to a THz pulse, whose electric field can couple directly with the order parameter linked to ferroelectricity. We wish to use light excitation to control the electronic state and take advantage of the coupling with the change of symmetry to control the ferroic properties by light.

Supervision:

The thesis will be supervised by Elzbieta Trzop (Research Engineer) for the experimental crystallography part and by Eric Collet (Professor) for the conceptual part. This thesis will mobilize other skills of members within the ML department for advanced structural studies of phase transitions, symmetry breaking and local order (diffuse diffusion, 3DΔPDF analysis) and optical spectroscopy.

E. Trzop is in charge of crystallography equipment and has trained many trainees, doctoral students and post-doctoral students in X-ray diffraction. E. Collet has supervised around ten theses since 2008.

E. Trzop and E. Collet will co-supervise the thesis at 50%.

This thesis aims to train a doctoral student within the DML on advanced crystallography and to exploit the existing crystallography equipment at the Institute of Physics of Rennes. It is a question of taking advantage of our know-how and our skills in order to develop innovative research projects.

A recent article published in IUCr Journal underlined our leading role in the study of photo-induced phenomena by ultra-fast diffraction.

This PhD project will be carried out at the Institute of Physics of Rennes and will involve mobility to synchrotron and X-FEL. The work will also be carried out within the framework of the International Research Laboratory DYNACOM piloted by S. Ohkoshi at the University of Tokyo and E. Collet at the University of Rennes. In this context, mobility to Japan may also be planned.

Required skills and knowledge

Candidates must have knowledge of solid-state physics, crystallography, phase transition. Candidates should know different experimental spectroscopy techniques (optics or X-rays), or even X-ray diffraction. The candidate should be familiar with data analysis and treatment and have good knowledge of programing (Python or similar). Knowledge of very large research infrastructures such as synchrotrons and X-FEL will be appreciated.

Références :

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