Ferroelectric materials for efficient light harvesting applied to solar cells

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If ferroelectric (FE) materials are largely used in microelectronic devices because of their dielectric properties, they are also particularly interesting for data storage, electrostrictive transducers and actuators, or pyroelectric heat detectors. The novelty during the last years is their integration in optoelectronic devices which includes photovoltaic (PV) solar cells. The key property of these materials is given by their internal electric field which is related to their intrinsic polarization. In PV cells integrating FE absorbers, the charge separation occurs because of this internal field which can exceed by far the one of a standard p-n junction. Such cells can therefore exhibit open circuit voltages much larger than the one expected by considering the bang gap width of the FE material. This allows expecting large power conversion efficiencies if charge generation and extraction rates exceed the recombination one. Thus, the main challenges towards the development of FE materials for PV applications are the control of the bandgap width (often larger than 2.5 eV) and the growth of high quality crystalline films, with no disordered phases and defects that can favor charge recombination.

We propose to tackle these challenges by studying the correlation existing between growth and optoelectronic properties at local (few tens of nm) and macroscopic (few cm) scales. We have chosen Bi_2FeCrO_6 (BFCO) as a model FE oxide which presents a gap of 1.5 eV if Fe and Cr are perfectly ordered. Although essential for the performance of solar cells, the Fe-Cr order was never accurately controlled and estimated.

In this project, an original methodology is developed for the detailed analysis of local properties aimed at structure, ferroelectricity and transport in BFCO thin films in order to identify and understand the key parameters that can lead to the improvement of the performance of solar cells incorporating FE absorbers. These properties will be modulated by controlling the order on the B/B' sites of the double perovskite structure via substrate-induced stresses. At the local scale, the characterisation will be done by near-field microscopy (PFM, CAFM) under dark or monochromatic light (variable wavelength hv-CAFM). This will allow to identify the role of defects (e.g. grain boundaries, O gaps), grain size, FE domain walls, stresses, as well as the role of different electrodes (metals and oxides) on the optoelectronic properties. Extensive structural characterisation of layers and interfaces will also be carried out. Resonant X-ray diffraction is a very powerful technique to determine precisely the cationic order between the B-B' sites and will be used for this purpose. Additional details on the order, crystal structure and interfaces will be obtained by transmission electron microscopy, and indirectly through magnetic and XPS measurements. The bandgap width will be determined from UV-visible absorption measurements. In parallel, electronic structure calculations will be carried out in order to explain the optoelectronic and magnetic properties measured experimentally or, conversely, to suggest relevant choices in terms of electrodes to be used in PV devices. The best solutions resulting from local optoelectronic measurements and ab initio calculations will be tested to realize macroscopic devices.

We look for a dynamic cadidate (master level), with strong personal motivation and solid background in physics, solid state chemistry or materials science. Good knowledge of English is desirable. He/she will be involved in the deposition of thin films, structural, and transport characterisation, as well as in the fabrication and testing of solar cells. IPCMS will actively promote the career of a successful PhD candidate within the relevant research communities through the participation in national and international conferences.