Poster

A multipurpose diffractometer for advanced SC-XRD experiments under T, P, E and h□

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Multifunctional materials combine in a single high tuneable system a set of different remarkable properties, controllable by distinct stimuli. Owing the strong structure/properties interplay in these materials, a detailed structural study is a prerequisite to shed light on the microscopic origin of their properties and design strategies to optimize their functionalities. To this purpose, it is mandatory to be able to probe the structure at the physical and time scales relevant for the properties of interest.

Single-crystal X-ray diffraction (XRD) is well celebrated technique for exploring structural changes on an atomic or even sub-atomic scale. But, when a state exists for a very short time or under than application for an external perturbation, an accurate and complete mapping of the reciprocal space can become very challenging, requiring news technical development and the implementation of a dedicated methodology.

It is in this context that we have developed a unique instrument for carrying out time-resolved photo-crystallography measurements as well as XRD measurements under a switched electric field. This diffractometer consists of a STOE STADIVARI II 4-circle goniometer and a Cegitek RebirX hybrid pixel detector. The experimental set-up developed synchronises a switched electric field or pulsed laser with the positioning of the goniometer and the detection of X-rays by the RebirX detector. The diffraction frames recorded are multiplexed and summed directly in the detector using firmware designed specifically for these experiments. The configuration using a switched electric field has been tested on quartz and also on a molecular compound. Finally, the diffractometer is complemented by a device for optical measurements (absorption, luminescence). The configuration with an Euler circle allows the use of complex sample environments such as a diamond anvil cell. The first measurements of photoluminescence under pressure on a hybrid perovskite have been carried out.