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Local Probing Energy Efficient Perovskites

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Naturally layered perovskite phases such as the Ruddlesden-Popper present an inspiring route to achieve unique magneto-electric, ferroelectric–photovoltaic or negative thermal expansion effects, among others. In these structures, the rotations of the disconnected perovskite octahedra can lead to different symmetry groups, polar and non-polar, and different magnetic orders adding extra pathways to engineer novel and efficient perovskite materials. Here, nanoscopic probing with local selective electrical and magnetic output information, is fundamental, as lattice distortions at the origin of the functional properties, do not always show clear macroscopic signatures. Of particular interest is to understand how the individual lattice modes evolve across phase transitions and within a particular symmetry. These symmetry-related fine details can be monitored via precise hyperfine Perturbed Angular Correlation γ-γ (PAC) measurements as recently reported [1, 2]. In these perovskites, specifically in $Ca_{3-y}Cd_yMn_{2-x}Ti_xO_7$, the MnO_6 octahedra rotation and tilting modes couple to polar cation displacement modes, inducing a ferroelectric polarization in a mechanism known as hybrid improper ferroelectricity [3-5]. Also, the negative thermal expansion observed in the lower dimension layered perovskite, e.g. Ca_2MnO_4, is associated with a MnO_6 antiphase rotation mode. PAC experiments performed in perovskite paradigmatic examples in a wide temperature range and obtained at ISOLDE-CERN will be presented. The evolution of the electric field gradient, EFG, combined with ab-initio electronic structure calculations are presented to show the EFG sensibility to distinct MnO6 distortion modes and how it can inform about the local details that govern macroscopic effects.

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