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Local Probing of Structural Phase Transitions in Naturally Layered Perovskites: $Li_2SrNb_2O_7$ as a case study

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Naturally layered perovskites have become an impressive playground for the birth of novel multifunctional devices due to its great electronic tunability aiming at innovative alternatives for improved energy storage devices and electronics. In particular, the search for room temperature ferroelectrics (FE) and magneto electrics has seen a boost in research focused on these structures. However, an accurate structural characterization at a microscopic scale can be notably difficult to establish by conventional scattering experiments [1], leading to conflicting reports in the literature. Our case study is the $n = 2$ pseudo Ruddlesden Popper (pRP) $Li_2SrNb_2O_7$, an interesting anti-FE and weak-FE system where the structural phases for functional applications are not yet fully understood with temperature [2,3].

Through Perturbed Angular Correlation (PAC) Spectroscopy measurements conducted at CERN/ISOLDE using ^{111m}Cd radio-isotopes, we can probe Hyperfine Interactions, in particular the local Electric Field Gradients at the Li and Sr lattice sites, commonly inaccessible to other techniques. With the help of ab-initio Density Functional Theory (DFT) calculations, we can establish the local effects that reproduce our measurements and that allow for the presence of switchable ferroelectric polarizations, granting us the fundamental understanding required to design new and optimal multifunctional materials.

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References:

[1] Rocha-Rodrigues, P. et al. Phys. Rev. B 101, 064103 (2020);
[2] Uppuluri, R. et al., Chem. Mater. 31, 4418–4425 (2019);
[3] Nagai, T. et al., Chem. Mater. 31, 6257–6261 (2019).

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