



Contribution ID: 22

Type: Talk

# Revealing the KDP soft-mode coupling mechanism with infrared spectroscopy under pressure

Wednesday 22 November 2023 11:00 (30 minutes)

Potassium dihydrogen phosphate,  $\text{KH}_2\text{PO}_4$  (KDP), is a classic, broadly used ferroelectric material. It is a model system of an order-disorder material, with a Curie temperature  $T_C$  of 123 K. Above this temperature, it is a tetragonal paraelectric. Below, it becomes orthorhombic. In the 1940s, Slater wrote an order-disorder theory to describe rather well the physics of KDP [1]. However, his theory failed to describe why the polarization doesn't change below the ordering temperature, and why  $T_C$  increases when hydrogen is replaced by deuterium. Therefore, it was understood that phonons must also play a role, through coupling to the proton which tunnels in a double well potential [2]. How exactly this happens remained unclear for a long time [3].

In our work, which spanned more than a decade and took place across two continents, we measured the far-infrared reflectivity of KDP up to 2 GPa in its ferroelectric and paraelectric phases. We identified an infrared mode that couples the hydrogen network to the lattice modes, to create the ferroelectric polarization.

[1] J. C. Slater, Theory of the Transition in  $\text{KH}_2\text{PO}_4$ , The Journal of Chemical Physics 9, 16 (1941).

[2] J. Pirene, On the ferroelectricity of  $\text{KH}_2\text{PO}_4$  and  $\text{KD}_2\text{PO}_4$  crystals, Physica 15, 1019 (1949).

[3] P. Simon and F. Gervais, Phase-transition mechanism in  $\text{RbH}_2\text{PO}_4$ -type ferroelectrics, Phys. Rev. B 32, 468 (1985).

**Primary authors:** AKRAP, Ana (University of Fribourg); HOMES, Christopher (National Synchrotron Light Source II, Brookhaven National Laboratory); SANTOS, David (Department of Physics, University of Fribourg); CAP-ITANI, Francesco (Synchrotron Soleil); LOBO, Ricardo (ESPCI Paris); NASRALLAH, Serena (Department of Physics, University of Fribourg)

**Presenter:** AKRAP, Ana (University of Fribourg)

**Session Classification:** Morning Session