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

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Potassium dihydrogen phosphate, KH_2PO_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 KH_2PO_4 , The Journal of Chemical Physics 9, 16 (1941).

[2] J. Pirene, On the ferroelectricity of KH_2PO_4 and KD_2PO_4 crystals, Physica 15, 1019 (1949).

[3] P. Simon and F. Gervais, Phase-transition mechanism in RbH_2PO_4 -type ferroelectrics, Phys. Rev. B 32, 468 (1985).

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