Poster Presentation

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Defect induced forbidden X-ray reflections in RbH2PO4.

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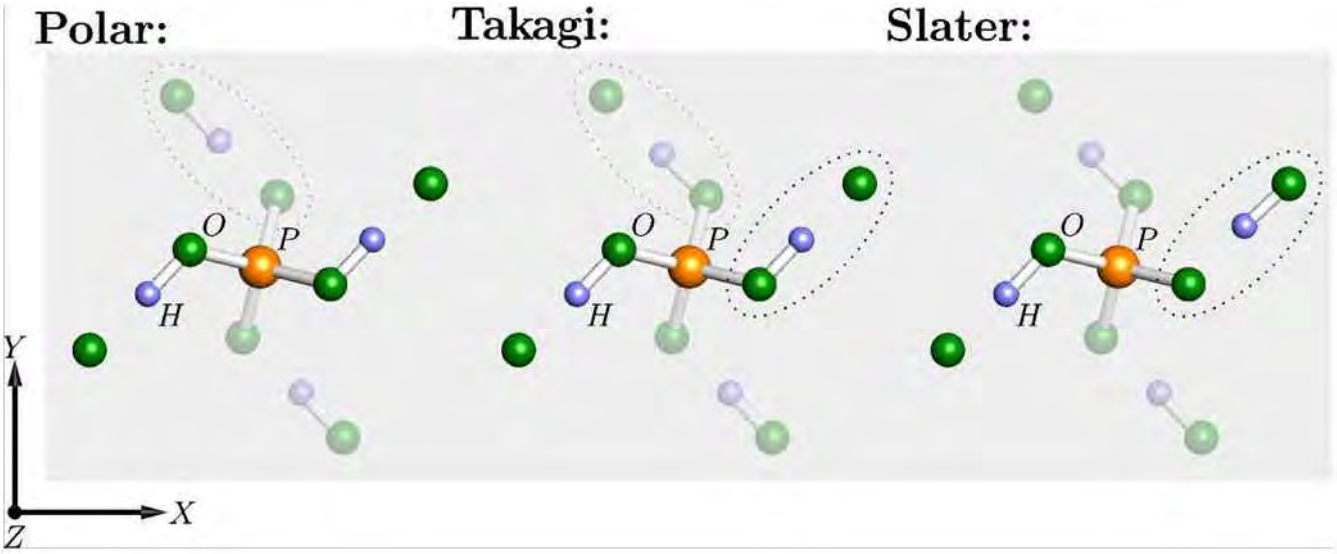
Resonant X-ray diffraction was used to study the proton jumps in hydrogen-bonded rubidium dihydrogen phosphate (RDP) crystals. In the paraelectric RDP phase, hydrogen is delocalized between two crystallographically equivalent positions. At lower temperatures, this symmetry can be broken, which defines the processes that lead to the para- to ferroelectric phase transition. We have measured the energy spectra of the forbidden reflections 006 and 550 at incident radiation energies close to the Rb K-edge in a wide temperature range, down to the temperature of the ferroelectric phase transition. In the paraelectric phase we observed a growth of integrated intensity for both forbidden reflections with temperature. This behavior is opposite to conventional non-resonant Bragg reflections, where the intensity decreases in accordance with the Debye-Waller factor. The developed theoretical model explains this effect with the thermal motion induced (TMI) scattering mechanism and also confirms the adiabatic approximation stating that electrons instantly follow the nuclei movements. In the 550 energy spectra, we have observed an additional contribution to the resonant structure factor which could be associated with the presence of transient Slater-type proton configurations (PC) in the half-filled hydrogen position.



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