

Delving into uncharted territories in the phase diagram of ferroelectric KNbO₃

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In the spirit of celebrating the synergy between Institut Néel and the ESRF, we turn our attention to a classic yet curiously underexplored ferroelectric material KNbO₃. This is a deceptively simple perovskite that conceals a remarkably rich pressure–temperature phase diagram, featuring a cascade of ferroelectric and paraelectric phases: rhombohedral *R3c* (R), orthorhombic *Amm2* (O), tetragonal *P4mm* (T), and the cubic paraelectric *Pm-3m* (C) parent phase [1]. Using high-pressure x-ray diffraction at room temperature in conjunction with Raman scattering up to 63 GPa, we unveil two previously unreported high-pressure phases. At 37 GPa, KNbO₃ transforms into a centrosymmetric tetragonal phase (*I4/mcm*). The phase is characterized by the appearance of superlattice reflections at $\mathbf{q} = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, indicative of octahedral tilts and a symmetry deviation from the cubic perovskite analogous to the behavior observed in EuTiO₃ [2]. Upon further compression to 44 GPa, we detect an incommensurate phase that transcends conventional perovskite behavior and reveals a complex interplay between lattice instabilities and octahedral rotations under extreme conditions [3].

[1] P. Pruzan, et. al, Vibrational dynamics and phase diagram of KNbO₃ up to 30 GPa and from 20 to 500 K, *Phase Transitions* 80, 1103 (2007).

[2] D. Bessas, et.al, Pressure-mediated structural transitions in bulk EuTiO₃, *Phys. Rev. B* 98, 054105 (2018).

[3] M. B. Shoker, et.al, An underdog story: Re-emergence of a polar instability at high pressure in KNbO₃, arXiv: 2508.06399 [cond-mat.mtrl-sci], (2025).