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Theoretical study of ferroelectric KNO_3 OSWALDO DIEGUEZ, Massachusetts Institute of Technology, DAVID VANDERBILT, Rutgers University — We present a detailed study of the structural behavior and polarization reversal mechanism in phase III of KNO_3, an unusual ferroelectric material in which the nitrate groups rotate during polarization reversal. This work extends a preliminary study presented as an example in our earlier paper on the mapping of the energy (E) versus polarization (P) in insulators.[1] Here we analyze in detail a two-parameter model in which the energy of the system is written as a low-order expansion in the polarization and in the nitrate group orientation. Apart from confirming that this model reproduces very well the first-principles results for KNO_3 presented in Ref. [1], we construct its parameter-space phase diagram, and in particular we describe regions of parameter space in which the $E(P)$ curves have an unusual triple-well structure. We also present first-principles calculations of KNO_3 under pressure, finding that as the material is compressed its $E(P)$ curves change character, going from having continuous to having discontinuous first derivatives at zero polarization.

[1]O. Diéguez and D. Vanderbilt, Phys. Rev. Lett. **96**, 056401 (2006).

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