

Abstract Submitted
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Constrained polarization study of ferroelectric KNO_3 ¹ OSWALDO DIÉGUEZ, DAVID VANDERBILT, Rutgers University — Potassium nitrate has an interesting phase diagram that includes a reentrant ferroelectric phase (phase III, $R3m$), and it has been proposed as a promising material to be used in random-access memory devices.² Recently, we have developed a method to compute the ground-state of an insulator under a fixed value of its polarization³ that can be used to gain insight into the properties of polar materials. In this talk we show the results of applying this method to study the structural behavior of potassium nitrate under polarization reversal, describing an unusual mechanism in which the reversal is accompanied by a rotation of the NO_3 unit by 60° . We also use our calculations as a basis for constructing first-principles based models that can be used to gain a deeper understanding of the switching behavior of this material.

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²J. F. Scott, M. S. Zhang, R. B. Godfrey, C. Araujo, and L. McMillan, Phys. Rev. B **35**, 4044 (1987).

³See: cond-mat/0511711 (www.arXiv.org).

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