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First Principles Study of Phase Transformations in Polyvinylidene Fluoride V. RANJAN, NC State University, Raleigh, NC, MARCO BUONGIORNO NARDELLI, J. BERNHOLC, NC State University, Raleigh, NC, and CSMD, ORNL, TN — Polyvinylidene fluoride (PVDF) with a small concentration of chlorotrifluoroethylene (CTFE) has been observed to store very high energy [1] as compared to currently used polymers. Chain rotations within the PVDF crystal have been proposed as the reason behind the high energy storage. However, in a recent work, we suggested [2] that the ultra-high energy storage in P(VDF-CTFE) is due to an electric-field induced phase transition from the non-polar α to the polar β-PVDF. We have now determined a low-energy relaxation path from α- to β-PVDF which confirms this suggestion. Our first-principles calculations reveal an intricate relationship between the kinetics of the chain rotation and the phase transformatio

[1] B. Chun, Science **313**, 334 (2006).
[2] V. Ranjan, Phys. Rev. Lett. **99**, 047801 (2007).

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