Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Energetic Study of the Flip-flop Motion of P(VDF-TrFE)[1]
XUEWEN WANG, LEI CAI, JIANDI ZHANG, Florida International University, P. A. DOWBEN, University of Nebraska-Lincoln — Ferroelectric copolymer P(VDF-TrFE) has attracted significant attention in material science and technology due to its excellent electromechanical properties and easy manipulation of the individual monomer or monomer clusters resulting in the change of the such properties. Theoretical aspect of the switching dynamics of P(VDF-TrFE) has been investigated by using the density function theory and compared with experimental results. Through calculation, we find a simple flipping of the individual monomer with lower energy that involves no change of the bond length and the bond angle of –C–C–, –C–H–, and –C–F–. These consist with the experimental results obtained with STM. We compare the STM image before and after the flipping of the monomers. Except the observation of the lattice shift at the boundary, we find no other structure distortion and no change in the inter- and intra- chain spacing.

[1]Work supported by NSF CHE0415421 and DMR-0346826

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Date submitted: 03 Dec 2005 Electronic form version 1.4