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First-principles investigation of high energy density in PVDF copolymers V. RANJAN, LIPING LU, NC State U., Raleigh, M. BUONGIORNO NARDELLI, J. BERNHOLC, NC State U., Raleigh and ORNL, TN — PVDF and its copolymers exhibit excellent electromechanical properties and in the case of PVDF-CTFE also a very high energy density [1]. We have investigated the phase diagram of these systems and can quantitatively explain the observed energy density of PVDF-CTFE as due to a para to ferroelectric phase transition in a disordered, multidomain structure [2]. Our results show that pure PVDF prefers the α phase at zero field. Electric field lowers the free energy of the β phase, resulting in a structural phase transition at a sufficiently high field. Copolymer admixture lowers the critical field and eventually leads to an energetic preference for the β phase even at zero field. For PVDF-CTFE with CTFE content below 17 %, the α phase is still preferred and the field-induced phase transformation reversibly stores large amounts of energy. For PVDF-TeFE, the total energy difference between the two phases is much smaller, resulting in substantially smaller energy density. [1] B. Chu et al., Science 313, 334 (2006). [2] V. Ranjan et al., PRL 99, 047801 (2007).

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