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**Mechanisms for achieving high energy density in PVDF: a first-principles investigation** V. RANJAN, NC State University 27695-7518, L. YU, MARCO BUONGIORNO NARDELLI, J. BERNHOLC, NC State University, Raleigh, NC 27695-7518 — It is known that copolymers of vinylidene fluoride (VDF) with about 50 – 80 % VDF fraction favor the polar  $\beta$ -phase, and these copolymers exhibit a paraelectric phase transition below the melting point. However, a larger concentration of VDF prefers a non-polar  $\alpha$ -phase. We have used first-principles calculations to determine the stable phases of chloro-tri-fluoroethylene (CTFE)-VDF mixtures. Our results show that a phase transition occurs in this system as a function of the electric field, leading to a very high energy density in P(VDF-CTFE)-based capacitors. Our results for polarization, dielectric constant, and energy density are in excellent agreement with earlier experiments [1] and provide a microscopic explanation for the formation of high energy density phases in P(VDF—CTFE) and similar polymer mixtures. [1] B. Chu et al., Science 313, 334 (2006).

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