Abstract Submitted
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**Microscopic mechanism of energy storage in PVDF-CTFE from ab-initio calculations** V. RANJAN, NC State University, Raleigh, NC, MARCO BUONGIORNO NARDELLI, J. BERNHOLC, NC State University, Raleigh, NC and CSMD, ORNL, TN — Polypropelene is most used capacitor dielectric for high energy density storage. However, exotic materials such as copolymerized Polyvinylidene fluoride (PVDF) could potentially lead to an order of magnitude increase in the stored energy density [1,2]. In contrast to linear dielectric properties of polypropelene, several polymers in the PVDF family display nonlinear dielectric properties under electric field. The nonlinearity was postulated to be due to a phase transition from non-polar to a polar structure, whose energy is lowered by an electric field [2]. Our calculations map out the atomistic details of phase transformations for both pure PVDF and PVDF-CTFE. Interestingly, admixture of a small amount of copolymer lowers both the polarization and the energy barriers for the transformation. The barrier lowering facilitates the transformation and may result in reduced loss in the charge-discharge cycle, enabling tuning of material properties for energy storage applications.

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

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