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Ab-initio study of high energy storage in polymers: PVDF-BTFE RUI DONG, V. RANJAN, North Carolina State Univ., M. BUONGIORNO-NARDELLI, Univ. of North Texas and Oak Ridge National Laboratory, J. BERNHOLC, North Carolina State Univ. and Oak Ridge National Laboratory — Previous experiments [1] and our theoretical work [2] have indicated that introducing CTFE monomers in polyvinylidene fluoride (PVDF) in small concentration can lead to ultra high density capacitive energy storage. Our previous work indicates that this is due to (i) formations of domains with different impurity concentrations, and (ii) existence of a low energy barrier path connecting ground state non-polar phase to a polar phase. We are now investigating bromo-triflouroethylene (BTFE) in a PVDF-BTFE as a potential high energy density material. Our results show that PVDF-BTFE prefers the nonpolar phase up to a higher concentration of 33%, as compared to PVDF-CTFE(17%). This could lead to a higher proportion of PVDF sample being available for phase transition under the electric field. The calculated energy barriers for the electric-field-induced phase transition are also low and comparable to PVDF-CTFE. We will discuss the calculated phase equilibria and the potential of PVDF-BTFE for high density capacitive energy storage.

[1] B. Chu et al., Science 313, 334 (2006).
[2] V. Ranjan et al., PRL 108, 087802 (2012); PRL 99, 47801 (2007).

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