

Abstract Submitted  
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**Theoretically guided design of efficient polymer dielectrics**<sup>1</sup> PHILIP TAYLOR, ELSHAD ALLAHYAROV, Case Western Reserve University — We have used theory and molecular dynamics simulation as an aid to the development of polymeric materials with favorable properties for energy storage with low dielectric losses. We build on the principle that the stored energy in a capacitor is a sum of the intrinsic energy of the electric field and the energy of distortion of the molecular bonds within the dielectric. We have attempted to maximize the energy of bond distortion by increasing the polarization without introducing large losses. In this initial study we simulate the behavior of a system consisting of parallel chains of the antiferroelectric  $\alpha$  phase of polyvinylidene fluoride that has been modified to increase the separation between chains through crosslinks that prevent chain rotation. By varying the crosslink density, we identify the optimum length of unlinked chain such that the polar entities that rotate when subject to a strong electric field will be neither so long that they rotate collectively with little stored energy, nor so short that the large distortion of bond angles necessary for dipole rotation reduces the polarizability. We have adopted a combined-atom model in order to make feasible the study of systems comprising up to 100 chains, each consisting of up to 500 monomers.

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