

Abstract Submitted
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Theoretical considerations in the design of polymer dielectrics¹

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Case Western Reserve University — An ideal dielectric is one that reversibly stores a large amount of energy when exposed to a modest electric field. 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. Because the stored energy in a capacitor resides mostly in the energy of distortion of the molecular bonds within the material, it is necessary to optimize the size of the deformable polar units. We achieve this by modeling some of the copolymers of polyvinylidene fluoride, and identifying the preferred density and nature of the cross-linking that pins certain regions of the polymer chains to prevent their rotation when exposed to fields. We then relate this to the electrostatic interactions within chains and between chains in order to take account of the depolarizing fields. We find the optimal length of chain between pinning points to be a function of the applied field strength, and to vary from about ten monomer units at the highest of fields to over a hundred monomers at very weak fields.

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