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Multiscale Modeling of the Electrocaloric Effect in PVDF-based Polymers ALAN MCGAUGHEY, YING-JU YU, Carnegie Mellon University — We apply multi-scale modeling to explore the electrocaloric (EC) effect in PVDF-related ferroelectric polymers, which have application in active cooling of microsystems. The EC effect is the temperature rise and drop in some ferroelectric materials due to changes in the configurational entropy when an external electric field is applied and removed. The polymer is modeled as a series of bi-directional permanent dipoles and induced point dipoles distributed on its monomer sites. The flipping of these dipoles due to an applied electric field is leads to polarization changes. Flipping the dipole moment of the polymer chain requires rotation of the individual monomers, each of which has its own energy barrier. This energy pathway is predicted from atomic-level nudged elastic band method calculations for a variety of chain environments. We then use first-passage time analysis to convert each energy pathway into an average transition rate for a full polymer chain rotation. The transition rates for all chains are integrated into a kinetic Monte Carlo algorithm in which the polarization change due to the application of an electric field is determined.

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