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First principles studies of self-polarization in electroactive polymers SERGE NAKHMANSON, Rutgers University, MARCO BUONGIORNO NARDELLI, NC State University, JERRY BERNHOLC, NC State University — The efficiency and physical transparency of the Wannier function formalism makes it especially suitable for studies of polarization and piezoelectricity in large systems ($>$ 100 atoms). We have used this approach to examine the polar properties of polyvinylidene fluoride (PVDF) and its copolymers with tri- and tetrafluoroethylene in different VDF-to-copolymer ratios. In the former case the monomer dipole moment is increased by 50% (from 2 to 3 Debye) as the isolated PVDF chains are brought together to form a crystal. In PVDF crystals containing copolymers we observe polarization enhancement, compared to pure PVDF, at copolymer concentrations of 10-16%. In general, our calculations show that polarization in electroactive polymers is described by cooperative, quantum-mechanical interactions between polymer chains, which cannot be viewed as a superposition of rigid dipoles.

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