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First-principles investigation of PVDF and its copolymers V. RANJAN, LIPING YU, North Carolina State University, Raleigh, NC, MARCO BUONGIORNO NARDELLI, J. BERNHOLC, North Carolina State University, Raleigh, NC and Oak Ridge National Laboratory, TN — Recently, PVDF and its copolymers have generated significant interest due to their electroactive properties [1] and potential for ultra-high energy-storage applications [2]. In this talk, we present the results of first-principles calculations of stable phases and dielectric properties of different copolymers and terpolymers of PVDF at varying concentrations. Our results show that at very high concentrations of Chloro-trifluoroethylene (CTFE), PVDF/CTFE displays sharp transitions between non-polar (α) and polar (β) phases. On the contrary, the same transitions in copolymers with trifluoroethylene (TrFE) and tetrafluoroethylene (TeFE) are not sharp and happen at lower concentrations. We discuss the interplay of copolymer admixture on the dielectric properties of PVDF and discuss the suitability of copolymers for energy storage and electroactive applications. [1] S. G. Lu et al., App. Phys. Lett. 93, 042905 (2008). [2] V. Ranjan et al., Phys. Rev. Lett. 99, 047801 (2007).

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