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**Dielectric Properties of Carbon, Silicon and Germanium Based Polymers: A First Principles Study** CHENCHEN WANG, GHANSHYAM PILANIA, CHUNSHENG LIU, RAMPI RAMPRASAD, University of Connecticut — The field of high energy density capacitors would benefit from the discovery of new insulating polymers with high dielectric constant, low loss, large band gap and high breakdown strength. The current standards for capacitive energy storage applications are polypropylene and polyethylene which have large band gap and high breakdown strength, but a small dielectric constant. As an initial step aimed at the discovery of new polymers with better dielectric properties, we consider a class of chemically-modified polymers based on polyethylene. These polymers are composed of –$XY_2$– building blocks, with X = C, Si or Ge, and Y = H, F or Cl. We use density functional perturbation theory and exchange-correlation functionals that include van der Waals and/or nonlocal exchange interactions to accurately predict the structure, dielectric constant (electronic and ionic) and band gap of this class of polymers. The computed properties have been correlated to the underlying electronic structure and phonon modes, and tradeoffs between the band gap and dielectric constant are established. The time-consuming dielectric computations have been optimized using a new "single-chain" method to allow for future extensive explorations of the polymer chemical space via automated high-throughput computations.

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