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Exploration of the Chemical Space of Group 4 Polymer Dielectrics CHENCHEN WANG, GHANSHYAM PILANIA, RAMPI RAMPRASAD, University of Connecticut — The current standards for capacitive energy storage applications are polypropylene (PP) and polyethylene (PE) which have large band gap and high breakdown strength, but a small dielectric constant. The envisaged next generation dielectric should provide high dielectric constant, while still preserving the insulating characteristics of PP and PE. To meet these growing needs, we use high throughput density functional theory (DFT) calculations in combination with machine learning (ML) methods to identify classes of polymers with large dielectric constant and band gap. In our work, we consider various possible local chemical modifications to polyethylene (PE). To be specific, we allow the -CH_2- unit in the PE backbone segment to be replaced by -SiF_2-, -$SiCl_2$-, -GeF_2-, -$GeCl_2$-, -SnF_2-, or -$SnCl_2$- units in a systematic manner. High throughput methods were used first to accurately determine the dielectric constant and band gap of the chemically modified PE chains for a set of limited compositions and configurations. ML methods were then used to predict the properties of systems spanning a much larger part of the configurational and compositional space. A set of most promising PE modifications (with simultaneously large dielectric constant and band gap) is identified using this strategy.

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