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Rational computational design of high energy density capacitor dielectrics through navigation of the polymer chemical space[1] GHANSHYAM PILANIA, CHENCHEN WANG, CHUN-SHENG LIU, R. RAMPRASAD, University of Connecticut — Next generation capacitor dielectrics should provide an attractive combination of high dielectric constant, fast response, low dielectric loss, high breakdown field and high temperature stability. With these objectives in mind, we adopt a research strategy in which newly developed high throughput first principles computational techniques are used to rapidly, and accurately, navigate the polymer chemical space to identify promising candidates. After validating our high throughput approach against computationally expensive dispersion corrected density functional theory calculations, we systematically study a number of C, Si and Ge backbone containing polymers with various side chain functional groups. Our initial accomplishment is the identification of new class of polymer systems with a large dielectric constant, and band gap large enough to provide reasonable insulating properties. These predictions are currently being validated by parallel experimental work, and are being further refined.

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