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Organotin polymeric dielectrics for energy-storage applications HUAN TRAN, ARUN KUMAR, CHENCHEN WANG, AARON BALDWIN, RUI MA, GREGORY SOTZING, RAMPI RAMPRASAD, Department of Materials Science and Engineering, Institute of Materials Science, University of Connecticut, 97 North Eagleville Road, Storrs, CT 06269 — We present a first-principles study on a family of organotin polymers which are based on -COO-$Sn(CH_3)_2$-OCC-$(CH_2)_n$ as the repeating unit (here $n = 0 - 10$). Among several members of this family which were recently synthesized, poly(dimethyltin glutarate) (corresponding to $n = 3$), is a promising candidate for high energy-density materials.[1] Given that the composition of each polymer is provided, we use the minima-hopping method to predict their stable structures. While the structural motifs predicted for these polymers are observed in several related existing polymers, other calculated physical properties, e.g., band gap E_g and dielectric constant ϵ, agree well with the experimental data obtained for the synthesized members. Comparing to polypropylene, the standard material for high energy-density applications, these polymers have smaller calculated E_g but significantly higher calculated ϵ. Overall, this whole family of organotin polymers are all promising for the purpose of capacitively storing energy. Our work is supported by the Office of Naval Research through the Multidisciplinary University Research Initiative (MURI).

[1]A. Baldwin *et al.*, submitted.

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