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First-principles design of organo-Sn polymeric dielectrics 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 — Following on from recent computation-based suggestions that Sn-containing polymers may be promising dielectrics, one of them, poly (dimethyltin glutarate) (pDMTG), has been synthesized. The measured dielectric constant of pDMTG is $\epsilon \simeq 7.4$, significantly higher than the current standard material used for high-energy-density applications, namely, polypropylene ($\epsilon \simeq 2.2$). By performing first-principles calculations at the level of density functional theory and using the minima-hopping method to predict the stable structures (given that just the composition is provided), we propose four structural models of pDMTG. Based on these models, various physical properties of pDMTG, e.g., dielectric constant, infrared spectra and refractive index, are determined to closely agree with experimental data. The calculated band gap of pDMTG is high ($E_{\rm g} \simeq 6.1$ eV), implying that pDMTG is a promising candidate for high-energy-density materials. The strategy that has lead to the synthesis and understanding of pDMTG shows that density functional theory is a powerful method to study and design new materials. Our work is supported by the Office of Naval Research through the Multidisciplinary University Research Initiative (MURI).

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