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**Tin-based inorganic-organic hybrid polymers for high energy-density applications** HUAN TRAN, ARUN KUMA, GHANSHYAM PILANIA, RAMPI RAMPRASAD, Department of Materials Science and Engineering, Institute of Materials Science, University of Connecticut, 97 North Eagleville Road, Storrs, CT 06269 — In one of our recent works<sup>1</sup>, an organotin polymer was synthesized and suggested to be promising polymeric dielectric, simultaneously exhibiting a high dielectric constant  $\epsilon$  and a high band gap  $E_g$ . Motivated by this result, we study a family of inorganic-organic hybrid polymers based on  $-(\text{SnF}_2)_x-(\text{CH}_2)_y-$  as the repeating structural unit ( $x = 2, y = 4, 8, \text{ and } 12$ ). The stable structures of these hybrid polymers, predicted by the minima-hopping method, are studied by first-principles calculations at the level of density functional theory. Our calculations show that these polymers are wide band gap materials (up to 6.07 eV). In addition, their dielectric constants are between 4.6 and 7.8, well above that of polypropylene ( $\epsilon \simeq 2.2$ ), the standard dielectric material for high energy-density capacitors. Therefore, we suggest that the hybrid polymers based on  $-(\text{SnF}_2)_x-(\text{CH}_2)_y-$  are promising candidates for high energy-density applications. Our work is supported by the Office of Naval Research through the Multidisciplinary University Research Initiative (MURI).

<sup>1</sup>A. Baldwin *et al.*, submitted.

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