First-Principles Studies of sila-Diamondoids

STEVEN L. RICHARDSON, Howard University, RAJENDRA R. ZOPE, TUNNA BARUAH, University of Texas at El Paso, MARK R. PEDERSON, Naval Research Laboratory — While there has been recent progress in the isolation of carbon-based diamondoids from petroleum oil by the Chevron-Texaco group, there is still no experimental evidence for the existence of the silicon analogue of adamantane, sila-adamantane (Si_{10}H_{16}). As adamantane forms the central building block for diamondoids, we speculate that sila-adamantane could serve as the template for a novel class of materials known as sila-diamondoids. We predict that because sila-diamondoids are nanostructures derived from bulk crystalline silicon they will have important applications in molecular electronics and nanotechnology. Recently, Fischer, Baumgartner, and Marschner (Science 310, 825 (2005)) have made an important contribution to the field of sila-diamondoids with the synthesis of a four-fold silylated molecule, C_{24}H_{72}Si_{14}. In this work, we show that density-functional theory is capable of calculating the structural, electronic, and vibrational properties of C_{24}H_{72}Si_{14} that compare very well with the recent experimental data.

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