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First-Principles Studies of sila-Diamondoids[1] 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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