Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

First-Principles Studies of the Electronic and Vibrational Properties of *sila*-Diamondoids[1] STEVEN RICHARDSON, UROS NOVAKOVSKI, Howard University — Diamondoids are cage-like, stable, saturated hydrocarbons, which possess a rigid carbon-framework that is superimposable upon the diamond crystal structure. These carbon-based diamondoids could be important building blocks in a variety of applications in biochemistry and nanotechnology. While the chemistry of silicon is not as robust as that of carbon, silicon-based analogues of diamondoids such as *sila*-adamantane ($Si_{10}H_{16}$) do exist and there is reason to believe that larger sila-diamondoids might either be synthesized in the lab one day or observed experimentally in chemical vapor deposition (CVD) experiments. In this work we show that density-functional theory (DFT) can accurately compute the electronic, structural, and vibrational properties of a variety of lower and medium-order *sila*-diamondoids. We believe that DFT is an important tool that will assist experimentalists in identifying more complicated *sila*-diamondoids that either may be synthesized or already may exist as important intermediates in CVD experiments to grow silicon surfaces.

[1]We wish to thank the Boeing Corporation for partial financial support of this research.

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Date submitted: 27 Nov 2009 Electronic form version 1.4