Materials Science and Technology Division

Materials Theory Seminar

"First-Principles Calculations of Diamondoids"

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Tuesday, January 30, 2007
11:00 a.m.
Third floor Conference Room, Bldg. 3025M

Abstract:
Diamondoids are cage-like saturated hydrocarbon molecules that possess a rigid carbon framework which is superimposable upon crystalline diamond. While lower-order diamondoids (e.g. adamantane ($C_{10}H_{16}$), diamantane ($C_{14}H_{20}$), triamantane ($C_{18}H_{24}$), and *anti*-tetramantane ($C_{22}H_{28}$)) have been synthesized in the lab, attempts to make even larger diamondoids have not been successful to date.

This field has recently been rejuvenated with the fascinating report by Dahl *et al.* of Chevron-Texaco (J. E. Dahl, S. G. Liu, and R. M. K. Carlson, *Science* **299,** 96 (2003)) of the isolation of new diamondoids from petroleum oil. Given the rigid structures and unique shapes of diamondoids they might be potential building blocks for various applications in nanotechnology and biochemistry. Recently, the Chevron-Texaco group also isolated and characterized a novel, disc-shaped lower-order diamondoid named cyclohexamantane ($C_{26}H_{30}$).

It is well known that density-functional theory (DFT) is a very successful approximation for solving the Schrödinger wave equation for real materials. DFT has been used in physics and chemistry for the last forty years and it can be implemented on modern massively parallelized supercomputers to compute the structural, electronic, magnetic, and vibrational properties of real materials and molecules from first-principles, that is without any experimental input. In particular, we will show that DFT calculations are quite capable of providing important information about cyclohexamantane and that our results are in very good agreement with recent experimental vibrational data. We are confident that DFT could assist experimentalists in identifying more complicated carbon-based diamondoids and other inorganic diamondoids (e.g. *sila*-diamondoids, BN-diamondoids) that can either be isolated from natural products or made by rational synthesis.

Steven L. Richardson, Tunna Baruah, Michael J. Mehl, and Mark R. Pederson, *Chem. Phys. Lett.* **403,** 83 (2005).

Steven L. Richardson, Tunna Baruah, Michael J. Mehl, and Mark R. Pederson, *Diamond Relat. Mater.* **15,** 707 (2006).

Host: David Singh