
COLLOQUIUM OF THE COMPUTATIONAL MATERIALS SCIENCE CENTER
College of Science
(CDS Department CSI 898-Sec 001)

"Modeling carbon based systems in nanoscience: from fullerenes and nanotubes to vacancies and pores in diamond."

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This talk will focus more on the challenges of modeling these diverse systems with various methods. Carbon is present in various materials in different hybridizations. We present a selection of modeling problems involving CC bonding.

Various molecular species exist in the relatively inert environment inside carbon nanotubes. These can be linear carbon chains, small molecules or larger molecules as fullerenes. We study structural, chemical bonding and vibrational properties of these species. Vibrations of a carbon chain inside nanotubes present unique challenges because of sensitivity to basis set, method choice and the need to include an extended number of neighbors in the calculation. We discuss the challenges and successes in validating the choice of the methodology used for our modeling.

Aspects of the microscopic mechanism of carbon nanotube actuation will be also discussed using ab initio modeling. We also discuss our new project on modeling the large pores in some porous carbon phases where the number of structural degrees of freedom are very large preventing the application of ab initio methods.

Monday , October 15, 2007
4:30 pm
Room 301, Research I, Fairfax Campus

Refreshments will be served at 4:15 PM.

Find the schedule at www.cmasc.gmu.edu/seminar/schedule.html