

Materials Science and Technology Division
and
Computer Science and Mathematics Division

**“Physics and Chemistry of Carbon materials: New
insight from *ab-initio* calculations”**

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Thursday, May 19, 2011
11:00 a.m.
4515/HTML, Room 265

Abstract

Carbon has a major role in our life. Carbon based fuels still provide most of our energy while new carbon materials appear as promising candidates for several technological applications. Despite their relevance, several aspects of Chemistry and Physics of Carbon materials remain poorly understood.

In this seminar I will present several *ab initio* electronic structure studies aimed at understanding fundamental interactions and chemical reactions in Carbon-bearing systems. The problems investigated represent prototype examples of present challenges for electronic structure methods. I will first review recent progresses in understanding weak interactions in graphite materials using *ab initio* many-body theory [1]. In particular I will show variational and diffusion quantum Monte Carlo calculations for the equilibrium interlayer binding energy in graphite. The behavior of the total energy as a function of interlayer separation will be discussed, comparing QMC results with the prediction of random phase approximation and other DFT-based approaches.

The second part of the seminar will be focus on physical and chemical properties of carbon fluids at high pressure and temperature. I will present free energy calculations and molecular dynamics results on the synthesis of higher hydrocarbon in the Earth mantle [2]. I will discuss the range of stability of pure methane and how the interaction with transition metals or carbon deposits (graphite and diamond) affects the formation of higher HCs

[1] L. Spanu, S. Sorella, G. Galli *Phys. Rev. Lett.* (2009) **103** 196401

[2] L. Spanu, D. Donadio, D. Hohl, E. Schwegler, G. Galli *PNAS* 2011 **108** (17) 6843-6846

Host: Fernando Reboredo (MSTD) and Bobby Sumpter (CSMD)