UNH Materials Science/Chemistry Joint Seminar

11:10-12:00, Thursday, October 16, 2008
Parsons Iddles L103, University of New Hampshire

Nanoscale Carbon: Large Acenes, Fullerenes and Carbon Nanotubes

Prof. Glen P. Miller
University of New Hampshire

A combined experimental and computational study of a series of substituted pentacenes including halogenated, phenylated, silylethynylated and thiolated derivatives will be presented. Experimental studies include the synthesis and characterization of six new and six known pentacene derivatives and a kinetic study of each derivative under identical photo-oxidative conditions. Structures, HOMO-LUMO energies and associated gaps were calculated at the B3LYP/6-311+G**//PM3 level while optical and electrochemical HOMO-LUMO gaps were measured experimentally. The combined results provide for the first time a quantitative assessment of HOMO-LUMO gaps and photo-oxidative resistances for a large series of pentacene derivatives as a function of substituents. With this substituent effect data in place, it is now possible to rationally design larger, photo-oxidatively persistent acenes. Two new persistent heptacene derivatives will be described.

Because acenes and cyclacenes map directly onto zig-zag carbon nanotubes, they can be considered precursors to semi-conducting single walled nanotubular compounds (SWNCs). We are interested in exploring this approach as a means to prepare a library of uniform SWNCs. Experimentally, a highly diastereoselective Diels-Alder reaction involving fullerenes has been demonstrated. Its potential utility to convert large acenes into cyclacenes will be discussed. Computationally, it will be shown that the electronic properties of SWNCs prepared by tethering cyclacene compounds vary as function of the tether.

Finally, a recently discovered chemistry for the hydrogenation of nanostructured carbons will be discussed. Fullerenes, SWNTs, MWNTs and graphite have all been successfully functionalized using this new chemsitry.

Host: Professor Jim Krzanowski x2315