ΕΘΝΙΚΟ ΜΕΤΣΟΒΙΟ ΠΟΛΥΤΕΧΝΕΙΟ
ΣΧΟΛΗ ΧΗΜΙΚΩΝ ΜΗΧΑΝΙΚΩΝ

ΕΠΙΤΡΟΠΗ ΣΕΜΙΝΑΡΙΩΝ, Καθηγητής Α. Κοκόσης

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ΣΕΜΙΝΑΡΙΟ ΧΗΜΙΚΗΣ ΜΗΧΑΝΙΚΗΣ

Τρίτη 14 Ιουνίου 2011, 13:00
Αίθουσα Σεμιναρίων «Ν. Κουμούτσου»

Professor **Mark C. Thies**

Department of Chemical Engineering
Clemson University

The Molecular Design of Advanced Carbon Materials: Synergism between Experiment and Molecular Modeling

The focus of Dr. Thies's current research program is on Experimental Thermodynamics and Separations, with an emphasis on supercritical fluids. Currently funded research topics are (1) Lignin Recovery and Purification from Waste Biomass Streams and (2) Structural Characterization and Quantitative Analysis of Carbonaceous Pitches.

Over the past two years, Thies's group has made significant strides in Project 2 above. In particular, their unique, 2-step separation technique of supercritical/dense-gas extraction followed by prep-scale, high-temperature GPC has enabled them to isolate the individual species present in petroleum pitches. These species were subsequently identified using advanced characterization techniques, including MALDI mass spectrometry and HPLC/UV-vis spectroscopy. A key finding of this work is that petroleum pitches consist of alkylated polycyclic aromatic hydrocarbon (PAH) monomers, dimers, trimers, and tetramers, with the degree of alkylation (0-6 methyls/monomer unit) being approximately Gaussian in distribution. The various aromatic backbones comprising the monomers were unequivocally identified, and the oligomers were found to consist of monomer units joined by a single, 5-membered ring.

With the success of the above experimental program in determining, for the first time, the molecular structures of the species present in petroleum pitch, Thies and co-workers are initiated the development of a molecular modeling effort for the prediction of the liquid crystalline properties of petroleum pitches as a function of oligomeric composition. Liquid crystalline petroleum pitches "designed" on the molecular level have outstanding potential as inexpensive precursors for advanced carbon materials, e.g., high thermal conductivity carbon fibers and graphenic systems.