Aug 19, 2011 10:40 AM Room 2124 EB3	**Dr. Jaehoon Kim** Korea Institute of Science and Research

Supercritical Fluids: New Opportunities for Energy Material Synthesis and Energy Production

Supercritical fluids can offer environmentally benign and facile synthetic conditions for the production of nanomaterials owing to their unique physical properties, including low viscosity, fast diffusion, zero surface tension, and tuneable physical properties. These factors make it a promising medium for overcoming the barriers associated with other techniques, which include the generation of toxic reaction waste, difficulty in producing nanosize materials, and transport limitations.

This talk will discuss various energy material synthesis and energy production using supercritical fluids. The energy material section will cover lithium iron phosphate ($LiFePO_4$), lithium titanium oxide ($Li_4Ti_5O_{12}$), and graphene synthesis in supercritical water or in supercritical alcohol for lithium 2nd battery applications.

The second part, the energy process section, will discuss current studies of hydrogen production in supercritical water, biooil production, and 2nd generation biodiesel production using supercritical fluids.

Aug 22, 2011 10:40 AM Room 1011 EB1	**Dr. Nicolas Buchler** Duke University

Building a Genetic Transistor in Yeast

Ultrasensitive, threshold responses are critical for robust bistability and oscillation in regulatory networks. Protein sequestration, where an active protein is bound in an inactive complex by an inhibitor, is a common molecular mechanism in natural regulatory circuits. Here I use a synthetic genetic circuit in budding yeast to show that sequestration of a basic leucine zipper transcription factor (C/EBPa) by a dominant-negative inhibitor converts a graded transcriptional response into a sharply ultrasensitive response, with apparent Hill coefficients up to 12.
A simple quantitative model for this genetic network shows that both the threshold and the degree of ultrasensitivity depend upon the abundance of the inhibitor, exactly as we observed experimentally. The abundance of the inhibitor can be altered by simple mutation; this suggests that responses mediated by protein sequestration are easily tunable.

Aug 29, 2011 10:40 AM 1011 EBI	**Dr. Andreas Bommarius** Georgia Institute of Technology

Development of a Biocatalyst for Stability & Selectivity

Biocatalysts command increasing interest in a variety of industries owing to their activity and often unsurpassed selectivity under mild conditions. As the design rules of biocatalysts begin to be understood, their development can proceed with fewer resources such as time and library size. Some of the most important trends are smaller, targeted libraries of variants, with restricted codons, the use of computational tools, and mechanism-based models for protein stability.

The first of two examples of biocatalyst development covers ene reductases/nitroreductases, which catalyze the reduction of C=C-, C=C-NO_2, or nitro moieties. Surprisingly, the stability of these flavoenzymes is limited by total turnover rather than thermal instability. Single variants, differing in just one amino acid residue, can cause big changes in enantioselectivity or substrate specificity.

The other example deals with cofactor-regenerating enzymes glucose dehydrogenase (GDH) and formate dehydrogenase (FDH), which need to be very stable for use in processes. Rational models point to the cause of their instability, such as interfaces or chaotropicity. Structure-guided consensus enabled enhancement of stability of GDH by one-million-fold. A perspective of biocatalyst development discusses goals for the next 10-20 years.

This joint seminar between BTEC and CBE is the 4th annual D. F. Ollis Lecture in Biochemical Engineering.

Sep 12, 2011 10:40 AM Room 1011 EB1	**Dr. Xiao-Dong Zhou** Dept. of Chemical Engineering, University of South Carolina

Oxygen Electrodes in Non-equilibrium Thermodynamic States

Equilibrium, is the situation when an energy system (e.g. a fuel cell or a battery) is under open circuit voltage. For cases that are not at equilibrium, but are close to it, Onsager established linear reciprocal relationships between flux and thermodynamic force. These linear relationships are manifested in transport phenomena, such as ion diffusion and heat conduction.

However, if an electrochemical reaction takes place at the electrode of a fuel cell or battery, the thermodynamic system is in a non-equilibrium, non-linear regime. As a result, in an active electrode the electrochemical reaction on the surface causes all thermodynamic variables to change in both the surface and the bulk.

In this seminar, I will use the oxygen electrode in fuel cells and lithium-air batteries as an example to address three questions related to materials in non-equilibrium thermodynamic states: (i) how do fast kinetics and high current in an operating fuel cell affect the thermodynamic states of its material constituents, (ii) whether or not the state of non-equilibrium can remain stable with constant flow of matter and energy, and (iii) what are the electrode materials that can be designed from theoretical studies?

In addition, I will briefly describe material physics and solid-state electrochemistry in four research areas that are being pursued in my group: (1) high rate electrodes in lithium-ion batteries for transportation use, (2) the electrocatalysts for carbon dioxide reduction, (3) thermoelectric oxides, and (4) defect chemistry.

Sep 19, 2011 10:40 AM Room 1011 EB1	**Dr. Constantine Megaridis** University of Illinois at Chicago (UIC)

Hierarchically Structured, Liquid-Repellent, Multifunctional Coatings with Tunable Properties

The behavior of fluids encountering hierarchically structured solid surfaces has been receiving significant attention recently. We present a polymer composite large-area coating method designed to impart desirable surface functionalities (such as super-repellency) to different substrates ranging from glass and metals to nonwoven materials and filters.
The wet-based approach relies on combining a polymer matrix in solvents with other materials to enhance adhesion and allow micro/nanoparticle filler dispersion. The advantage of the technique lies in its inherent ability to impart multiple functionalities by adding the proper ingredients to the solution, which is deposited on the target surface by spray or other techniques. The approach combines tunable surface energy with micro-to-nano scale roughness, a necessary condition for *super-repellent*behavior.
In some coatings, super-repellency is combined with self-cleaning ability, which is effected by low droplet roll-off angles. We demonstrate thin coatings with controllable micro/nanostructure, hydrophobicity, and electromechanical properties, combined with good mechanical or environmental durability. Several examples (including elastomeric, electrically conducting and icephobic coatings) are given to show the potential of this method for select technological applications.

Sep 26, 2011 10:40 AM Room 1011 EB1	**Dr. Ramanan Krishnamoorti** University of Houston

Lipid-based Anti-Inflammatory Drug Delivery

Nonsteroidal anti-inflammatory drugs are one of the most widely consumed pharmaceuticals, yet the mechanisms involved in their therapeutic actions and side-effects, notably gastrointestinal ulceration/bleeding have not been clearly defined. We have used a number of biochemical, structural and computational systems to demonstrate that NSAIDs have a strong affinity to form ionic and hydrophobic associations with zwitterionic phospholipids that are reversible and non-covalent in nature.
We propose that the pH-dependent partition of these potent anti-inflammatory drugs into the phospholipid bilayer, and possibly extracellular mono/multilayers present on the luminal interface of the mucus gel layer, may result in profound changes in the hydrophobicity, fluidity, permeability, biomechanical properties and stability of these membranes and barriers.
These changes provide an explanation of how NSAIDs induce surface injury to the GI mucosa as a component in the pathogenic mechanism leading to peptic ulceration and bleeding. This insight has proven useful in the design and development of a novel class of PC-associated NSAIDs that have reduced GI toxicity while maintaining their essential therapeutic efficacy to inhibit pain and inflammation.

Oct 3, 2011 10:40 AM Room 1011 EB1	**Dr. Randy K. Avent** Dept. of Computer Science, NCSU
The Role of Computational Sciences in Strategic Growth Areas	
As data proliferates, connections grow and predictive analytics become more important, computational sciences become an increasingly important field in most research domains. This talk will provide insight on the role of computational sciences in the Defense Department and will present a strategic roadmap for investments. Other important areas like biotechnology, manufacturing and analytics will be summarily discussed as well.	

Oct 10, 2011 10:40 AM Room 1011 EB1	**Dr. Alexander Deiters** Dept. of Chemistry, NCSU
Synthetic Chemical Tools for the Regulation of Cellular Processes	
We are developing parts for the expansion of the genetic code of pro- and eukaryotic organisms with synthetic amino acids, in order to provide new function to cells and proteins. Our main focus is on generating light-activatable proteins through the site-specific incorporation of photocaged amino acids in bacterial and mammalian cells. The genetic code expansion is achieved through the engineering of cells with an orthogonal tRNA/tRNA synthetase pair, and the evolution of the corresponding synthetase to only accept the photocaged amino acid as a substrate. In order to achieve excellent light-activation characteristics of the proteins of interest, we rationally select amino acid residues in active site locations, based on mechanistic and crystallographic data. This approach was applied to the photochemical control of DNA recombination, DNA polymerization, RNA polymerization, kinase function, zinc-finger nuclease activity, and sub-cellular protein localization. Using these tools we were able to generate bacterial and mammalian cells that respond to light with a distinct activation and deactivation of gene expression in a spatially and temporally restricted fashion.	

Oct 31, 2011 10:40 AM Room 1011 EB1	**Dr. Yaroslava Yingling** Dept. of Materials Science and Engineering, NCSU

Understanding Nucleic Acid Based Material Properties Through Molecular Modeling

Nucleic acids are appealing candidates for assembly of synthetic materials due to their versatility in function and structure and molecular recognition properties of base pairing. Using these properties DNA and RNA molecules have been engineered into novel nanostructures to make up various effective 2D and 3D nanoparticles, nanotubes, drug delivery capsules, and scaffolds for the assembly of molecules components.

We use molecular modeling techniques to provide a complete microscopic description of the structure and dynamics of NAs under different environmental conditions, from detailed information on atom-to-atom interactions with ions to global functionally important motions and conformational changes which control the processes of self-assembly.

In this talk, I will discuss the structure and properties of DNA functionalized on inorganics surfaces for biosensors, the interactions of DNA with nanoparticles and the folding of RNA into drug delivery devices. Fundamental advances in understanding the processes driving the self-assembly of complex nucleic acid molecules may further advance their use in nanotechnology and will allow us to build a more complete picture of the structure and functions of natural biomolecules.

Nov 7, 2011 10:40 AM Room 1011 EB1	**Dr. Brian Kuhlman** Dept. of Biochemistry and Biophysics, UNC - Chapel Hill

Computational Design of Protein Interfaces and Switches

Three stories in protein design will be presented:

(1) the design of a new conformation and sequence for a protein-binding peptide;

(2) the redesign of protein-protein interactions in the ubiquitin pathway using a computationally engineered library;

(3) the design of genetically encoded photoactivable proteins based on the LOV domain.

Central to all problems in protein design is the need to identify amino acid sequences that are compatible with a predefined target structure or binding interaction. To address this problem, we develop and use the molecular modeling program Rosetta.

The core methods in Rosetta for sequence and conformational optimization will be discussed.

Nov 14, 2011 10:40 AM Room 1011 EB1	**Dr. Gabriel P. Lopez** Triangle Materials Research Science & Engineering Center
Stimuli Responsive Polymers for Biotechnological and Biomedical Applications	
This talk will present studies of different types of stimuli responsive polymeric materials — including thermally, electrically and acoustically active materials — in the form of thin films and microparticles. We have developed active nano- and micro-structured thin films that allow dynamic control of specific and nonspecific attachment of biological molecules, cells and organisms. We are also developing acoustically active microparticles that can be used in microbioanalytical operations such as immunoassays and rare cell separations. The talk will emphasize areas of research that might naturally be suited for collaborative endeavor with soft materials researchers at NC State and across the Research Triangle in general.	

Nov 21, 2011 10:40 AM Room 1011 EB1	**Dr. Oleg Borodin** Army Research Laboratory
Insight into Electrolyte Structure from MD Simulations	
Design of electrolytes for secondary lithium batteries and supercapacitors is a complicated task as an electrolyte has to satisfy a number of often conflicting requirements such as low bulk and charge-transfer ionic resistance over a wide temperature range, low volatility and flammability, compatibility of the electrolyte with the separator and electrode materials. Molecular dynamics (MD) simulations and density functional calculations (DFT) have a potential to provide fundamental understanding of interfacial and bulk electrolyte properties. In this presentation I will discuss how MD simulations using recently developed APPLE&P polarizable force field aid in understanding of structural and transport properties of a wide range of electrolytes from traditional carbonate mixtures to ionic liquids and their interactions with electrodes. Charge transfer resistance known to dominate lithium battery impedance will also be examined by exploring the energetics of the lithium desolvation from electrolyte. Finally, electrolyte oxidative stability and decomposition pathways obtained from DFT calculations will be discussed.	

Nov 28, 2011 10:40 AM Room 1011 EB1	**Dr. Ashutosh Chilkoti** Dept. of Biomedical Engineering, Duke University

Elastin-like Polypeptides: New Motifs and New Self-Assembling Systems

This talk will describe new developments in the design, synthesis, self-assembly and application of stimulus responsive peptide polymers. The developments include:
1. Elastin-like polypeptides (ELPs) –a class of recombinant peptide polymers that display lower critical solution temperature transition (LCST) phase behavior in aqueous solution– to self-assemble into nanostructures in response to a range of stimuli. This approach of attachment-triggered encapsulation of small hydrophobic molecules into soluble nanoparticles has great utility to increase the solubility, plasma half-life and tumor accumulation of cancer chemotherapeutics.
2. Triple-responsive diblock ELPs that self-assemble into monodisperse micelles in response to a thermal trigger, that can be further stabilized by metal ion chelation within the core of the micelle and that disassemble in response to a small drop in pH.
3. Peptide polymers –syntactomers– that display LCST phase behavior, with a syntax that ranges from simple peptide repeats ("words"), to syntactomers that approach the sequence complexity of proteins ("phrases"). These syntactomers illustrate that syntax may be a useful concept in the design of peptide based polymers.
Recombinant peptide polymers provide rich opportunities for application in biotechnology and medicine, and a few applications of these biomacromolecules will also be highlighted in this talk.

Dec 12, 2011 1:00 PM Room 2018 - EB1	**Dr. Simeon D. Stoyanov** Unilever R&D The Netherlands

Foam Stabilization Using Shape-Anisotropic Biomaterials

The stability of aerated products is mainly limited by the disproportionation process. This problem can be partly avoided by gelling the continuous phase, but it can lead to undesired textural changes. The real solution is to structure (gel) the bubble surface, making it very elastic and impossible to shrink/expand.
As a result, there's broad interest in the study of solid particles as emulsifiers of dispersed systems. The advantage of particle stabilization is that it's almost impossible to displace a particle once it's adsorbed to an interface, which gives particle-stabilized foams excellent stability.
Here we will illustrate our approach to stabilization of emulsions and foams by using rigid CaCO3 rods modified by fatty acids. We will also describe our work using fibers made from ethyl cellulose or shellac wax, which can have additional functionality.
Finally, we will show how nature creates some of the most beautiful colours using light diffraction from colloidal structures, and how we use this approach to create colourful bubbles stabilized by mixtures of modified CaCO3 rods and modified pearlescent pigments.