

Aug 27, 2012

10:40 AM

Room 1011 - EB1

Professor Keith Weninger

Department of Physics – NCSU

***Conformational Dynamics Allow Repair Proteins to Detect DNA Mismatches***

The DNA mismatch repair system is critical for accurate DNA replication. This system is highly conserved across organisms ranging from bacteria to humans reflecting the importance of minimizing genomic defects during cell division.

The mismatch repair protein MutS has been identified as the key factor that detects base-base mismatches and insertion-deletion mismatches in double stranded DNA and signals for their repair. Despite intense study, a temporally resolved understanding of the molecular details of the MutS:DNA interactions during mismatch repair initiation has been difficult to obtain because these transient interactions occur within an overwhelming background of properly matched DNA basepairs.

We used single molecule fluorescence resonance energy transfer (smFRET) to characterize conformational changes in MutS as it scans homoduplex DNA, recognizes mismatches, activates to a sliding clamp, and interacts with downstream proteins in the repair signaling pathway. We found a series of sequential conformational changes that provide a mechanistic picture of: i) dynamic DNA bending by MutS, ii) concomitant conformational changes within MutS itself, iii) motion of MutS scanning along DNA, iv) ATP binding states that commit MutS:mismatch DNA complexes to convert to sliding states used in signaling, and v) the modulation of these MutS behaviors by other regulatory factors.

**Sep 10, 2012**  
**10:40 AM**  
**Room 1011 - EB1**

**Andreas Heyden**  
Dept. of Chemical Engineering - University of South Carolina

***Understanding and Designing Heterogeneous Catalysts from First Principles***

[Speaker's Website](#)

For heterogeneously catalyzed reactions with more than one key surface intermediate, it is likely that multiphase catalysts have a significant advantage over conventional monophase catalysts since each phase can potentially be adjusted independently to activate a key reaction step. At the same time, our understanding of bifunctional multiphase systems is relatively poor. It is the objective of the first part of this seminar to illustrate recent progress in understanding heterogeneous catalysis at the three-phase boundary of a gas-phase, a reducible oxide surface, and a noble metal cluster. In particular, we intend to illustrate the specific role of the three-phase boundary in determining the activity and selectivity of TiO<sub>2</sub> supported Pt catalysts for the water-gas shift (CO + H<sub>2</sub>O → CO<sub>2</sub> + H<sub>2</sub>) reaction.

One of the principle goals of modern catalysis research is to understand reaction mechanisms on solid surfaces to a degree that practical activity and selectivity descriptors can be identified that permit the rational design of new stable catalysts with unprecedented activity and selectivity. High selectivity towards a single reaction product is driven both by economics and the goals of green catalysis, where atom- and energy-efficient processes are required to conserve the world's limited resources. In the second part of this seminar we present a computational case study for the determination of activity and selectivity descriptors for the hydrodeoxygenation of organic acids to alkanes and olefins on transition metal surfaces relevant for the conversion of triglycerides to green diesel and hydrotreating (upgrading) of bio-oils obtained from pyrolysis of lignocellulosic biomass.

**Sep 17, 2012**  
**10:40 AM**  
**Room 1011 - EB1**

**Kenneth Schweizer**  
Depts. of Materials Science, Chemical & Biomolecular Engineering and Chemistry - University of Illinois @ Urbana-Champaign

***Theories of Soft Materials: From Polymer Nanocomposites to Nonequilibrium States of Dense Colloidal Suspensions***

[Speaker's Website](#)

A major goal in the statistical mechanics of soft materials is to understand and predict how the chemical and physical nature of individual macromolecular species and the thermodynamic state determine bulk structure, phase behavior, dynamics and properties. We have developed a microscopic equilibrium theory for polymer nanocomposites that addresses the critical roles of polymer-particle interfacial attraction, filler size and concentration, and solvent dilution on the collective structure, miscibility and bulk modulus of these hybrid nanomaterials. The key physical ideas and distinctive predictions will be presented, along with quantitative applications to scattering and viscosity experiments on hydrocarbon polymer-silica nanocomposites. The existence and size of stabilizing adsorbed

polymer layers, their consequences on spatial dispersion and microstructure, and nonclassical nanoscale effects on properties have been established based on a combined theory-experiment approach. An emerging area of particle science and engineering concerns the assembly, structural relaxation, rheology and kinetic arrest of dense suspensions of nonspherical colloids. We have developed microscopic statistical dynamical theories for the activated and coupled translation-rotation dynamics of dense suspensions of uniaxial colloids under quiescent and strongly deformed conditions. Criteria for the formation of nonequilibrium gels and glasses, and their elastic properties and stress-driven yielding behavior, have been studied. Predictions for how the competing repulsive and attractive forces and shape anisotropy lead to new types of nonequilibrium phase diagrams, two-step relaxation and unusual double yielding will be described, and quantitative comparisons to recent experiments presented. Most recently, the theory has been extended to dense mixtures of spheres and rods, systems of interest as novel inks for direct write printing applications and in various biophysical contexts. New dynamical complexity again emerges now triggered by large steric packing asymmetry.

**Sep 24, 2012**

**10:40 AM**

**Room 1011 - EB1**

**Christina Chan**

Dept. of Biochemistry and Molecular Biology - Michigan State University

***Integrative analysis to identify novel targets and to understand differentiation***

[Speaker's Website](#)

Our research focuses on understanding the molecular, signaling and cellular processes that are altered in diseases. The overall objectives of the group fall into two research directions. The first aim is to identify novel targets involved in diseases, i.e. cancer and Alzheimer's disease. This involves activities ranging from developing computational methods that integrate high throughput technologies to traditional molecular and cell biology techniques in the identification of novel targets. Here, I will briefly describe some of our work the application of computational modeling in identifying targets relevant to cancer. The second aim of the lab is to develop tools and approaches to ameliorate the disease, through targeted delivery or cell-based therapies; or preventing the disease through identification and characterization of molecular targets of known bioactive components involved in disease prevention. Along these lines I will discuss some of our research on the combined impact of chemical and mechanical stimuli on neural differentiation of mesenchymal stem cells (MSCs) and its implication for neurodegenerative diseases.

**Sep 27, 2012**

**2:15 PM**

**Room 1007 - EB1**

**Younan Xia**

Dept. of Biomedical Engineering; School of Chemistry and Biochemistry,  
Georgia Tech

***Complex Nanomaterials via Simple Chemistry***

[Speaker's Website](#)

The first documented synthesis of nanocrystals can be traced back to the beautiful work by Michael Faraday in 1856 when he demonstrated the preparation of gold colloids with a ruby color. Ever since, many different methods have been developed for preparing nanocrystals, but essentially all the products were troubled by problems such as irregular shapes, broad size distributions, and poorly defined morphologies. Only within the last decade has it become possible to generate nanocrystals with the quality, quantity, and reproducibility needed for a systematic study on their properties as a function of size, shape, and structure. I will briefly cover some of these developments in this talk, with a focus on solution-phase syntheses of noble-metal nanocrystals. While the synthetic methods only involve simple redox reactions, we have been working diligently to understand the complex physics behind the simple chemistry - that is, the nucleation and growth mechanisms leading to the formation of nanocrystals with well-controlled sizes, shapes and properties. The success of these syntheses has enabled us to tailor the plasmonic and catalytic properties of noble-metal nanocrystals for a range of applications including photonics, sensing, imaging, biomedicine, catalysis, and fuel cell technology.

**Oct 1, 2012**

**10:40 AM**

**Room 1011 - EB1**

**Anthony M. Dean**

Dept. of Chemical and Biological Engineering - Colorado School of Mines

***Free Radical Kinetics: From Diesel Ignition to Biocorrosion***

[Speaker's Website](#)

The improved understanding of elementary chemical reactions has markedly improved our ability to describe "real-world" systems. Such approaches require development of accurate, detailed chemical mechanisms, which in turn require careful analysis of different types of elementary reactions. This talk will describe our approach to the characterization of elementary reactions, the construction of detailed mechanisms, and the application to several systems, ranging from hydrocarbon oxidation to thermochemical biomass conversion to biocorrosion. We will focus on the development of rate rules for various types of free radical reactions and discuss how these can then be applied to begin to understand the impact of introducing various types of alternative fuels.

**Oct 8, 2012**

**10:40 AM**

**Room 1011 - EB1**

**Yiannis Kaznessis**

Dept. of Chemical Engineering and Materials Science - University of Minnesota

***Mathematical Models in Biology: From Molecules to Life***

[Speaker's Website](#)

A vexing question in the biological sciences is the following: can biological phenotypes be explained with mathematical models of molecules that interact according to physical laws? At the crux of the matter lies the doubt that humans can develop faithful mathematical representations of living organisms, doubt fed by the astonishing complexity of biological systems. However intense are the efforts of biologists to reduce organisms to sequences, structures and interactions, the difficulty to develop tractable mathematics hampers the connection between theory and reality in biology. We think there are two major reasons for this difficulty: First, biological systems are not only non-linear and often stochastic, but they possess an overwhelming number of variables. Consequently, although in principle these systems obey physical laws, there are insurmountable mathematical difficulties to develop meaningful, tractable, first-principles models. Second, biology is a discipline in history: Dobzhansky's dictum that "Nothing in biology makes sense except in the light of evolution" casts a long shadow on mathematical models of phenotypic complexity. Because, how exactly can we integrate thermodynamics with evolution?

Is there then any hope that mathematics will ever be considered as indispensable a tool in the biosciences as in the physical sciences? We think there is. We believe that a synthetic biology research program may liberate empiricism beyond the unaided human brain. Humans can now construct and piece together DNA sequences in order to design new biological systems and organisms. We can do this more quickly and less expensively than ever. Synthetic biology is the discipline that focuses on the construction of these novel biological systems.

Synthetic biological systems confer three advantages that may indeed help us make a plausible case for so ardent a vision, as to describe biology with mathematics: a) they are small and well-defined enough to be captured by universal yet tractable mathematical models; b) they are modular enough to string together and build logical and informational architectures that are the essence of living systems; c) they are to some extent our designs, not nature's, avoiding some of the difficulties of historical explanations.

Armed with supercomputers and sophisticated mathematical models we can then investigate how information is transferred from molecules and their interactions, to cascades of gene regulatory relations, to emerging logical and informational architectures in bacteria. In the presentation we will first discuss multiscale models of antimicrobial peptides to explore the tractability of mathematical models that are founded on universal laws of thermodynamics and principles of molecular biology. We will then discuss models of synthetic constructs and argue that computer simulations take on the role of tractable mathematics, bringing us one step closer to determining whether life's distinctiveness can be explained by the laws of chemistry and physics.

**References**

Volzing K, Biliouris K, Kaznessis YN. "proTeOn and proTeOff, New Protein Devices That Inducibly Activate Bacterial Gene Expression." ACS Chem Biol. 2011 Oct 21;6(10):1107-16

Kaznessis Y, "Mathematical models in biology: from molecules to life." Wiley Interdiscip Rev Syst Biol Med. 2011 May-Jun;3(3):314-22. doi: 10.1002/wsbm.142

Bolinteanu D, Kaznessis YN. "Computational studies of protegrin antimicrobial peptides: a review." Peptides. 2011 Jan;32(1):188-201

**Oct 22, 2012**

**10:40 AM**

**Room 1011 - EB1**

**Chuan-Hua Chen**

Dept. of Mechanical Engineering and Materials Science - Duke University

***From Jumping Drops to Thermal Diodes***

[Speaker's Website](#)

On superhydrophobic surfaces, condensate drops spontaneously jump upon coalescence, giving rise to self-sustained dropwise condensation without any external driving forces. The self-propelled motion results from the surface energy released upon drop coalescence, while the out-of-plane jumping results from the superhydrophobic substrate breaking the symmetry of energy release. In this talk, we will first illustrate the physical mechanism of the self-propelled jumping, including the capillary-inertial velocity scaling and the conditions conducive to the spontaneous motion. We will then discuss two applications of the jumping drops: a new self-cleaning mechanism for water-repellent surfaces that works without rain, and a planar phase-change thermal diode that is inherently scalable to large areas.

**Nov 5, 2012**

**10:40 AM**

**Room 1011 - EB1**

**Darrell Velegol**

Dept. of Chemical Engineering - Penn State University

***The Design of Self-swimming Colloidal Motors***

[Speaker's Website](#)

Colloidal motors are micron-sized particles, often consisting of metals such as platinum, gold, or silver. They can also be made of various minerals, such as calcium carbonate. The motors have the ability to consume chemical energy and move autonomously, often at >10 micrometers/sec. Not only can the motors self-move individually, but collections of the motors often give an emergent directed motion, much like bacterial populations that engage in chemotaxis or phototaxis movement. In this talk I will describe simple techniques for fabricating the motors or using existing minerals, examine the auto-electrokinetic mechanisms by which the motors move individually, and analyze how the motors communicate with each other and the system to achieve collective movement. Then we will explore several key challenges and opportunities with colloidal motors: How do we fabricate custom motors? How do we design and control their individual and collective transport? What is required for scaling up production of the motors? And might the auto-electrokinetic transport mechanism have important applications?

**Nov 12, 2012**

**10:40 AM**

**Room 1011 - EB1**

**S. Birgul Tantekin-Ersolmaz**

Dept. of Chemical Engineering - Istanbul Technical University

***Designing Membranes for Energy Efficient Gas Separations***

**[Speaker's Website](#)**

Energy efficient separation technologies are needed for long-term sustainability of the process industry. Polymeric membranes have been studied extensively for the past three decades for many gas separation applications ranging from CO<sub>2</sub> capture, air separation, and hydrogen purification to olefin-paraffin separation. However, the current polymeric membranes are still inadequate to fully supply the demand of high permselectivity for most of these applications. Inorganic materials such as zeolites and metal organic frameworks (MOF) can also effectively separate many gases. Although these materials have much higher potential separation efficiency than polymers, difficulties in their preparation in the form of large surface area modules and their cost have made them less attractive as membrane materials. Mixed matrix membranes (MMMs), typically composed of these selective inorganic particles distributed in a polymeric matrix combine the superior separation ability of the former and the ease of formation into larger defect-free modules of the latter. MMMs can fulfill further expectations when merged with the advances in nanotechnology for the synthesis of well-defined nanoscaled zeolites and MOFs with high reproducibility to enable the preparation of ultra thin membranes. Many factors including the physical properties of the polymer forming the matrix, and the inorganic particles, as well as the interaction between the particle and the polymer have a tremendous effect on the MMM performance, which is hard to predict prior to experimentation. Additionally, the solvent type used in MMM fabrication and thermal treatment conditions are among the parameters which may affect the gas permeation properties. This talk will describe our approach to designing MMMs for some important gas separation applications and explore several key challenges on the design path. We will focus on the interface characteristics and its influence on the membrane performance for different polymer-particle systems.

**Nov 19, 2012**  
**10:40 AM**  
**Room 1011 - EB1**

**Bridget Rogers**  
Dept. of Chemical and Biomolecular Engineering - Vanderbilt

***Synthesis and Characterization of Oxide-based Ceramic Phosphors***

[Speaker's Website](#)

Oxide-based ceramic phosphors have been used in TV's, displays, LED's, and as laser sources. Recent work at Vanderbilt by our group has suggested that these materials may also be used as passive radiation exposure indicators. This talk will discuss our work to synthesize several oxide-based phosphors and characterize the materials' chemical, physical, and optical properties.

We use combustion synthesis to produce the oxide-based ceramic phosphors. Combustion synthesis involves heating a mixture of metal nitrates and a fuel until the mixture ignites. If the proper conditions are used the energy released by the combustion is sufficient to form polycrystalline material. Combustion synthesis, in general, is a fairly established technique. However, we have found that the properties of the synthesized materials are strongly dependent on several process variables and conditions. Mixing of the fuel and oxidizers during heating is key to achieving ignition and a producing uniform batch of material. The rate at which the mixture is heated also was found to be critical in achieving ignition, as fuels can begin to decompose before the ignition temperature is reached. Even the size of the crucible used to perform the synthesis can affect the resulting material.

I will present results of our studies to understand the affects of process variables on the chemical, physical, and optical properties of combustion synthesized oxide-based ceramics. We used XRD to determine crystallinity and grain size of the oxides. XPS was used to determine the chemical composition and bonding within the oxides. Photoluminescent spectral intensities and peak positions was used to determine the optical properties of the oxides.

**Dec 3, 2012**  
**10:40 AM**  
**Room 1011 - EB1**

**Robert D. Kiss**  
Director, Late Stage Cell Culture - Genentech, Inc.

***Ollis Lecture: Biochemical Engineers Battling the Biological / Biochemical Challenges to Cell Culture Process Development and Manufacturing***

Biochemical engineers play key roles in the development of robust and productive cell culture manufacturing processes. The challenges keeping their jobs interesting and rewarding come in many flavors, including equipment/material interactions and incompatibilities, contamination risks, and process variability, and can result in process operational failures or product quality failures. Some of the biggest challenges have interesting biological/biochemical origins or root causes. This presentation will review experiences in managing these biologically-driven challenges (a.k.a., blame it on the cell culture) through cell line engineering, media and process condition optimization, and sound engineering approaches. Specific examples include preventing viral contamination, preventing catastrophic monoclonal antibody disulfide bond reduction, and reducing the levels of recombinant protein variants that can affect resultant product quality.