Jan 30, 2012 10:40 AM Room 1011 EB1	**Dr. Friedrich Srienc** Dept. of Chemical Engineering and Materials Science, University of Minnesota

Predicting the Evolution of Metabolic Networks

Ever since the process of natural selection was originally described by Charles Darwin and Alfred Russell Wallace, one question has captivated the minds of many: ‘‘how predictable is evolution?’’

It is generally recognized that even under constant selection, predicting evolutionary change is challenging for two main reasons. First, evolution is a complex mixture of deterministic and chance events. Second and most important, predicting evolution requires a detailed knowledge of the range of available mutations and their fitness effects.

We will discuss the analysis of metabolic networks for designing optimal pathways, and show that the network structure can be related to fundamental thermodynamic properties. This enables the prediction of mutations happening during adaptive evolution.

Feb 6, 2012 10:40 AM Room 1011 EB1	**Dr. Regina Murphy** Dept. of Chemical and Biomolecular Engineering, University of Wisconsin

Protein Misfolding and Aggregation in Neurodegenerative Diseases

Misfolding and aggregation of peptides and proteins has been linked to toxicity in Alzheimer’s, Huntington’s, and other neurodegenerative diseases. In Alzheimer’s disease, aggregation of the peptide Abeta and its subsequent deposition as fibrils are thought to be the underlying cause of neurotoxicity. In senile systemic amyloidosis (SSA), the protein that aggregates is the circulating transport protein, transthyretin (TTR).Recent studies support for the hypothesis that these two amyloidogenic proteins interact, and that this interaction is biologically relevant.

In this presentation I will describe our detailed examination of the association between TTR and Abeta. We have used several complementary techniques to identify specific interaction regions of TTR and Abeta, and have explored the role of quaternary structure in modulating TTR-Abeta association. Our results led us to propose that TTR is a natural anti-AD ‘drug’, and that its protective ability is somehow lost or attenuated with aging.

Feb 13, 2012 10:40 AM Room 1011 EB1	**Dr. John Pojman** Department of Chemistry, Louisiana State University

Cure-On-Demand Polymerizations

The goal of cure-on-demand polymerization is to create one-pot systems that have a long shelf live but will react rapidly when curing is desired. We use two approaches: coupling polymerizations with clock reactions and an approach called frontal polymerization in which a localized reaction zone propagates from the coupling of thermal transport and the Arrhenius dependence of the reaction rate of an exothermic polymerization.

We demonstrate that frontal polymerization can used to create a cure-on-demand putty for filling holes in wood, marble, and sheet rock. The putty has a months-to-years shelf life, is a one-pot formulation, can be applied leisurely and then cured rapidly with a flat heat source. We also demonstrate frontal polymerization can be used to create an adhesive for wood and plastic-wood composites that cures rapidly and has impressive shear strength. Finally, we will explore current efforts to commercialize "nerd putty" for the art market.

Feb 20, 2012 10:40 AM Room 1011 EB1	**Dr. Jennifer Reed** University of Wisconsin – Madison

Systems Approaches for Exploring and Exploiting Cellular Metabolism

Genome-scale networks of metabolism and regulation can be reconstructed from an organism's genome annotation. Models generated from these reconstructions can be used to integrate and analyze different types of experimental data in order to generate hypotheses about biochemical network structure, interactions between organisms and their environments, and responses to genetic and environmental perturbations.

Examples from modeling different bacteria with biotechnology and metabolic engineering applications will be presented to illustrate how modeling and experimental efforts can be combined to improve computational models and our understanding of cellular metabolism and regulation. Once accurate models are developed, computational tools can be applied to design microbial strains with enhanced chemical production.

We have recently developed new methods for proposing metabolic engineering strategies based on metabolic and regulatory model predictions. These strategies can involve transcription factor and metabolic gene deletions, as well as enzyme over expression. Using these approaches we have identified genetic strategies for improving production of a variety of biochemicals in *E. coli* including ethanol, isobutanol, succinate, amino acids, and malate.

Feb 27, 2012 10:40 AM Room 1011 EB1	**Dr. Erik Santiso** Imperial College London

Modeling the Nucleation Mechanism of Molecular Crystals from the Melt and from Solution

Understanding crystallization is crucial for many applications in the food, chemical and pharmaceutical industries. Despite its widespread use, however, the design of crystalline materials is far from an easy task. With the exception of a few simple systems, the molecular-level details of the nucleation process are still poorly understood. On the one hand, the stochastic nature of nucleation, and the fact that it usually involves only a few molecules/ions, make it very hard to probe experimentally. On the other hand, the time scales involved are beyond the reach of traditional molecular simulation methods.

In this work, we combine a novel method to characterize the degree of order in molecular crystals
[1] with the string method in collective variables
[2] to obtain minimum free energy pathways for the nucleation of several systems from the melt and from solution. We then use milestoning with Voronoi tesselations
[3] to obtain free energy barriers for nucleation. We compare some of the results from this approach with those obtained using transition path sampling.
Finally, we show how this method can be extended to study aggregation in systems where the aggregates only exhibit partial ordering. These results are a first step toward a molecular-level understanding of nucleation in molecular systems.

Mar 12, 2012 10:40 AM Room 1011 EB1	**Dr. Joseph Tracy** Materials Science and Engineering, NCSU

Synthesis, Self-Assembly, and Transformations of Metal and Magnetic Nanoparticles

Ligand-stabilized nanoparticles are of significant interest for their size- and shape-tunable physical properties, and the ligand monolayers facilitate self-assembly. New approaches for synthesizing and assembling nanoparticles and studies of nanostructural transformations within nanoparticles will be presented:
(1) the magnetic field-directed self-assembly of magnetic nanoparticles into chains in three dimensions,
(2) the nanoscale alignment of gold nanorods within macroscale-aligned electrospun polymer nano/microfibers,
(3) the process of void formation through the Kirkendall effect, when nickel nanoparticles are converted into nickel oxide or nickel phosphide,
(4) the sinter-free conversion of arrays of alloy FePt nanoparticles into intermetallic phases with analysis by scanning transmission electron microscopy, and
(5) a new synthetic approach for controlling the size of thiolate-stabilized gold nanoparticles that alters the magic sizes.

Mar 19, 2012 10:40 AM Room 1011 EB1	**Dr. Allen Foegeding** Food, Bioprocessing and Nutrition Sciences, NCSU

Designing Food Structure: Linking Chemistry, Physics and Biology

Food is essential for life ("eat to live") and often the central focus of our daily joys ("live to eat"). *Food structure* represents the assembly of molecules into structures observed at nano, micro and macroscopic scales.

The appearance, texture and stability of many foods are due to formation of sols, foams, emulsions, gels or glass structures during processing. Current demands for low caloric density, low sodium, low fat, low sugar, high omega-3 fatty acids and high fiber versions of traditional foods have highlighted the difficulty in *a priori* design of a desirable food structure.

We are operating on the basic hypothesis that: 1) food structure determines the breakdown pattern during oral processing and 2) the physiological sensations perceived during oral processing contribute to the cognitive representation of texture formed in the brain. We have been successful in establishing structure-texture relationships for properties that are based mainly on strength or deformability of materials. In contrast, properties derived from spatial or adhesive perception in the oral cavity are more difficult to explain based on food structure.

Implications to producing a healthy and sustainable food supply will be discussed.

Mar 26, 2012 10:40 AM Room 1011 EB1	**Dr. Xuanhe Zhao** Mechanical Engineering and Materials Science, Duke University

Engineering Soft Active Materials for a Better Life

The interaction of engineering and biology has created exciting opportunities for discoveries, inventions, and commercialization. At Duke Soft Active Materials Laboratory, we are transforming an essential feature of biology systems into engineering materials and devices, i.e. to receive stimuli from the environment and then move.

In this talk, I will focus on novel soft materials capable of giant deformations in response to electric and magnetic fields. The fundamental physics and mechanics for the active deformation of these materials will be first discussed. Thereafter, I will introduce novel applications of these materials in areas as diverse as energy storage, energy harvesting, drug delivery and anti-biofouling.

Finally, inspirations from nature and daily life are extremely useful in studying these novel materials and applications, and thus the inspirations from things such as lotus leaf, sharpie dog, aging skin and human lung will also be shared with the audience.

Apr 2, 2012 10:40 AM Room 1011 EB1	**Dr. Qibing Pei** University of California, Los Angeles

Transparent Composite Electrodes for Stretchable Polymer Thin Film Devices

Both single wall carbon nanotubes and silver nanowires have been employed to fabricate transparent electrodes by an in-situ composite synthesis and transfer technique. The composite electrodes retain the high conductivity of the conductive network and the mechanical flexibility of the polymer matrix. Surface roughness of the composites is less than 10 nm, suitable for the fabrication of thin film electronic devices.

The electrodes can be stretched by up to large strains without significant loss of sheet resistance. The composites are used to fabricate three flexible devices: (1) polymer LEDs, (2) polymer solar cells, and (3) bistable electroactive polymer actuators. The LEDs show 15-50% higher efficiency than control devices fabricated on ITO/glass substrate.
The solar cells exhibit lower efficiency than controls due to insufficient surface coverage. When a stack of short and long silver nanowires are employed in the composite, the photovoltaic performance is increased to being comparable to the controls. The composite electrodes have also been used for Joule heating and the actuation of polymer actuators to large strains.
I will additionally describe the fabrication of intrinsically stretchable polymer LEDs and refreshable Braille readers.

Apr 9, 2012 10:40 AM Room 1011 EB1	**Dr. Brian Davison** Oak Ridge National Laboratory

BioEnergy Science Center: An Integrated Strategy to Understand and Overcome Biomass Recalcitrance

The challenge of converting cellulosic biomass to sugars is the dominant obstacle to cost-effective production of biofuels. The BioEnergy Science Center (BESC) research program addresses this challenge with an interdisciplinary effort focused on overcoming the recalcitrance of biomass.

BESC research addresses (1) targeted modification of plant cell walls to reduce their recalcitrance, and (2) consolidated bioprocessing, which involves the use of a single microorganism or microbial consortium to overcome biomass recalcitrance.

This update will highlight BESC achievements. BESC has developed a high-throughput characterization pipeline to see how turning different plant genes on or off can cause cell-wall compositional and structural changes that affect enzyme deconstruction. This characterization pipeline is being utilized for both natural variants of switchgrass and Populus as well as transgenic strains.

One of the first genes in switchgrass that we modified has resulted in a 25% increase in ethanol production. We are also developing skills to manipulate and understand cellulolytic microbes which improve ethanol tolerance.

Apr 16, 2012 **10:40 AM** **Room 1011 EB1**	**Dr. Frances H. Arnold** California Institute of Technology

McCabe Lecture - Design by Evolution: Engineering Biology in the 21st Century

Biology could offer elegant solutions to human problems that range from producing fuels and chemicals from sunlight and carbon dioxide to combatting disease. The one proven algorithm for biological design—evolution—can compose the DNA that codes for these functions.
A powerful approach to creating useful new biological functions, directed evolution both circumvents and underscores our profound ignorance of how sequence encodes function. Where natural evolution has gone, directed evolution can follow. Even more interesting are the proteins nature may not have cared about, but biomolecular engineers dream of. I will describe some exciting applications of this approach to engineering the biological world.

Apr 23, 2012 **10:40 AM** **Room 1011 EB1**	**Dr. Hong Yang** University of Illinois at Urbana-Champaign

Materials Design of Bimetallic Catalysts for Electrochemical Energy Applications

Nanomaterials are important for the design of electrocatalysts for fuel cell and battery applications. In the past several years, low temperature hydrogen fuel cells for automotive applications have witnessed tremendous progress. Now the major automotive companies are gearing towards bringing the fuel cell hybrid vehicles (FCHV) to consumers in 2015. A major driving force for this rapid development lies in the rapid progress made for creating active cathode catalysts for proton exchange membrane fuel cells (PEMFC).
I will present our recent work on the design and solution-phase synthesis of Pt bimetallic and multimetallic nanostructures with controlled composition and shape, which are important structural parameters for electrocatalysis, including a new synthetic approach to the shape control of Pt alloys based on the gas reducing agent in liquid solution (GRAILS) method and using CO as reducing.
I will show the synthetic processes, underlying formation principles and advantages of using core-shell and other heterogeneous nanostructures. These structures are used for the design of catalysts. I will further illustrate the structure-property relationship in selective systems, such as {111} faceted Pt_3Ni nanocrystals and Pt-on-M (M=Ag, Au, Pd, etc.) electrocatalysts for oxygen reduction reaction (ORR) and fuel molecule oxidation reaction.