

Jan 26, 2009  
10:45 AM  
Room 1011, EB1 1

Dr. Jeffrey Elam  
Argonne National Laboratory

***Atomic Layer Deposition of Platinum on Strontium Titanate Surfaces***

Tremendous energy savings and environmental benefits are possible from improved catalysts for chemical manufacturing and emissions reduction. Breakthroughs in catalyst development will be enabled by precise methods for synthesizing nanostructured materials. Atomic layer deposition (ALD) is a thin film growth technique that is currently used by the microelectronics industry and offers great potential for synthesizing better catalysts.

In this seminar I will present recent results from work at Argonne synthesizing, characterizing, and testing materials comprised of ALD platinum on strontium titanate surfaces as potential catalysts for reducing automotive emissions. We employ a variety of analytical techniques including scanning- and transmission-electron microscopy, and synchrotron X-Ray scattering methods to understand the structure and composition of the platinum catalysts and also to explore the ALD growth behavior.

Surprisingly, the ALD Pt consists of nearly monodispersed nanoparticles that decorate the strontium titanate and are highly active for hydrocarbon combustion.

Feb 9, 2009  
10:45 AM  
Room 1011, EB1

Dr. Bryan W. Berger  
University of Pennsylvania School of Medicine

***Sequence, structure and specificity in transmembrane helix oligomerization***

Protein-protein and protein-lipid interactions in membranes govern important biological processes such as neurogenesis, viral fusion and cell adhesion. Common to each of these processes is the role of transmembrane domains in regulating the oligomeric state of the membrane receptors involved. This talk will focus on the sequence and structural features of transmembrane (TM) helix-helix interactions as well as design approaches used to probe their function.

Using a combined experimental and theoretical approach, we examined the role of TM domain interactions in the regulation of  $\beta_1$ - and  $\beta_3$ -integrins. Using scanning mutagenesis, we identified a novel "large-small" interaction motif for the isolated alpha/beta TM heterodimer that appears to be conserved across the integrin family. Mutations at key positions in this motif for the respective full-length integrins lead to constitutive activation in multiple transfected cell lines.

In a second approach, we used a recently developed computational method, CHAMP (computed helical anti-membrane protein), to design peptides that target the TM domains of membrane proteins in a sequence-specific manner. Furthermore, using genetic selection methods, we are able to examine the specificity and affinity of interactions between the designed and target TM helices for the multimeric M2 influenza channel.

Overall, our results indicate that TM peptides can be designed to selectively interact with a given target as well as how a CHAMP methodology can be generalized to examine a wide range of TM-mediated processes.

Feb 16, 2009  
10:45 AM  
1011 EB1

Dr. Jacinta C. Conrad  
University of Illinois at Urbana-Champaign

***Structure and flow of non-equilibrium colloidal suspensions***

Colloidal suspensions are ubiquitous in industrial and technological applications, and moreover serve as excellent model systems for a variety of complex fluids. In particular, the structure and flow properties of non-equilibrium suspensions are relevant for materials such as inks, coatings, paints, and personal care products.

In this seminar I will discuss three studies relating the structure of non-equilibrium colloidal suspensions to their flow properties. First, we use confocal microscopy to investigate relationships between structure and dynamics near the hard-sphere colloidal glass transition, one of the fundamental unsolved problems in condensed matter physics. By identifying slowly-relaxing regions within our samples, we show that the structure of these clusters is correlated to the macroscopic mechanical properties of the suspension.

Second, we use microscopy, light scattering, and rheology to characterize the properties of dense colloidal gels formed via arrested phase separation. These dense gels exhibit structural properties of both fractal colloidal gels and colloidal glasses, yet their mechanical properties are strikingly different from either.

Finally, we design model colloidal gels to mimic inks used for direct ink writing, a rapid prototyping techniques, and use microscopy to investigate their flow properties in microchannels. Both the extent of flow-induced structural disruption in the colloidal gel and the qualitative features of its flow profile are directly related to its bulk mechanical properties. Collectively, these measurements yield fundamental insight into the relationship between structure and dynamics in non-equilibrium colloidal suspensions, and provide guidance towards the design of improved materials for extrusion.

**Feb 18, 2009**  
**10:45 AM**  
**135 BTEC**

**Professor Theodore W. Randolph**  
University of Colorado at Boulder

***High Hydrostatic Pressures as a Tool to Recover Folded Protein From Aggregates and Inclusion Bodies***

Protein aggregates are a serious problem facing the biotechnology industry. During the production of recombinant proteins aggregation causes dramatically reduced process yields and heavy environmental costs.

Hydrostatic pressures between 1 and 3 kbar cause dissociation of multimeric proteins. At higher pressures, typically 5-10 kbar, monomeric proteins will unfold. There is thus a pressure “window” between about 2 and 5 kbar wherein the native state of monomeric proteins is thermodynamically favored, but multimeric proteins will dissociate into their subunits.

By applying pressures in the “window”, we dissolve the aggregates in a fashion similar to the dissociation of multimeric proteins, and concomitantly refold the protein because the native state is still favored. High yields of folded protein are obtained, and folding yields are independent of protein concentration at concentrations to 10g/L.

For protein aggregates containing disulfide-crosslinked aggregates, application of high hydrostatic pressures in the presence of disulfide shuffling agents produced higher yields of active protein than conventional, chaotrope-based refolding processes.

**Mar 9, 2009**  
**10:45 AM**  
**EB1, Room 1011**

**Chase L. Beisel**  
California Institute of Technology

***Engineering ligand control of RNA interference***

RNA interference (RNAi) is a powerful tool to silence gene expression in humans and other eukaryotes. The ability to specifically target any gene in the genome has revolutionized both basic biological research and opened new avenues in the treatment of inheritable and infectious diseases. A central challenge in both application areas is controlling the spatial and temporal activity of RNAi. To address this challenge, we have developed a generalized molecular framework for ligand control of RNAi.

In this talk, I will discuss the engineering of ligand-responsive shRNAs and miRNAs. I will show how structural insights into RNA processing and RNAi activation can be translated into the successful integration of ligand control. I will also discuss two important properties of any molecular framework, modularity and flexibility, that are both crucial when tailoring designs to the regulatory demands of a desired application.

Both properties are reflected by our generalized molecular frameworks, including the ability to readily swap aptamer domains and gene targeting sequences, and the ability to modify designs for tunable and combinatorial control of gene expression. Modified designs are based on structural and functional insights into naturally-existing miRNAs, establishing an important link between biological discovery and the elucidation of design principles for the successful construction and implementation of engineered biological systems.

Mar 11, 2009

3:30 PM

Room 2018, EB1

Professor Stavroula Sofou

Polytechnic Institute of New York University

***Lipid membrane heterogeneities controlled by pH: basic studies and potential applications***

Nature uses lipid membranes as a universal wrap around cells, and there is increasing evidence that it controls critical cell functions by reorganizing lipid membranes into rafts. Lipid-rafts are nanometer- to micron-size domains of laterally phase-separated lipids whose occurrence coincides with changes in the local cell surface topography, local multivalency, and membrane integrity.

These structural changes seem to correlate with cell functions including membrane trafficking, cell signaling, protein transport and viral infection mechanisms. The processes regulating these changes are largely unknown.

We use model lipid bilayers to study simplified processes that alter the surface topography of membranes, the apparent reactivity of surface-grafted functional groups, the membrane permeability and fusogenicity, with the aim to potentially contribute to the understanding and control of related cell functions and associated diseases. We design such basic pH-dependent processes on model functionalized lipid bilayers in the form of small unilamellar vesicles and giant unilamellar vesicles.

Integration of these processes on nanometer-sized lipid vesicles used as drug delivery carriers may precisely control their interactions with diseased cells increasing therapeutic efficacy while minimizing toxicities.

Mar 16, 2009  
10:45 AM  
1011 EB1

Dr. Guohui Wu  
University of California, Santa Barbara

***Structural Integrity of Lipid Membranes: Strategies for Membrane Sealing and Controlled Drug Delivery***

Biomembranes are essential to many biological functions. Despite its critical role in supporting life, the biomembrane can be damaged by traumas such as electrical shocks, frost bites, etc. Membrane sealing is thus an important topic in membrane biophysics.

We have conducted studies towards the understanding of the mechanism of membrane sealing. Our results show that the poloxamer, an effective sealing agent, selectively inserts into damaged membranes, thus localizing its effect on the damaged regions. The inserted poloxamer is "squeezed out" at tighter lipid packing, suggesting a mechanism for the cell to get rid of the poloxamers when the membrane integrity is restored.

On the other hand, biomembranes have important applications in drug delivery. Liposomes are essential bases of cell membranes and have been used as biocompatible lipid-based drug carriers.

An elusive goal for drug delivery is to provide both spatial and temporal control of contents release. We achieve this via a novel externally photo activated approach where hollow gold nanoshells (HGNs) are used as triggering agents.

Near-complete contents release from lipid carriers can be initiated within seconds by irradiating HGNs with a near-infrared pulsed laser. Other carriers, such as polymeric carriers could be modified with this approach for controlled release.

Mar 23, 2009  
10:40 AM  
1011 EB1

Dr. William M. Miller  
Northwestern University

***Challenges in Blood Cell and Platelet Production in Culture***

Stem cells in the bone marrow differentiate into the various blood cell lineages via several rounds of lineage-restricted commitment and cell expansion, followed by lineage-specific cell proliferation and maturation. Recovery of neutrophil and platelet counts determines the engraftment time after stem cell transplants, and can be accelerated by supplementing large numbers of culture-derived granulocytic and megakaryocytic (Mk) progenitor and post-progenitor cells.

More than 12 million units of red blood cells and 4 million units of platelets are transfused each year in the U.S. Production of red cells and platelets from cultured blood stem and progenitor (CD34+) cells would increase the supply of rare blood types and decrease the risk from blood-borne pathogens. However, major advances will be required for the development of clinical production processes.

We and others have demonstrated that blood cells can be successfully cultured in a variety of bioreactor systems. The main challenge is to identify conditions that allow for selective commitment to the lineage of interest, extensive cell expansion, and lineage-specific maturation. We are focusing on Mk cells and platelets.

We are developing a 3-step process with cytokines and environmental conditions tailored for each step. We used a factorial design to identify cytokines that produce at least 3 Mk progenitors (each of which can produce up to 50 Mk cells) per input CD34+ cell, while enriching the proportion of Mk progenitors. Understanding the mechanisms responsible for NIC-mediated increases in Mk ploidy will facilitate regulatory approval for using NIC to produce platelets for transfusions and is likely to lead to the discovery of even more effective conditions for Mk polyploidization.

Mar 30, 2009  
10:45 AM  
1011 EB1

Eranda Nikolla  
University of Michigan, Ann Arbor

***Electrochemical Energy Conversion: Molecular approaches toward the development of carbon-tolerant electrocatalysts for solid oxide fuel cell (SOFC) anodes<sup>1</sup>***

Dwindling fuel resources and high greenhouse gas emissions have increased the need for more efficient energy conversion systems. A promising technology relies on the electrochemical conversion of the chemical energy of hydrocarbons into electrical energy using solid oxide fuel cells (SOFCs). One of the main issues associated with the direct conversion of hydrocarbons on SOFCs is that conventional anode electrocatalysts, such as Ni on yttria-stabilized zirconia (YSZ), deactivate due to the formation of carbon deposits. We have utilized density functional theory (DFT) calculations to study carbon chemistry on Ni and Ni-containing alloy electrocatalysts. The main objective of these studies was to develop molecular insights regarding carbon poisoning on Ni and to utilize this molecular information to identify possible carbon-tolerant alternative anodes to Ni.

DFT calculations showed that certain Ni surface alloys had lower tendencies towards carbon poisoning as compared to monometallic Ni. The identified alloy catalysts have been synthesized and characterized using various spectroscopic and microscopic techniques. The potential utility of these alloy materials as carbon-tolerant SOFC anodes was experimentally demonstrated.

We have also probed the electronic structure of Ni and Ni alloys using electron energy-loss near-edge spectroscopy (ELNES), in-situ x-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy (AES). We show that even small changes in the near Fermi level electronic structure of Ni catalysts, induced by the formation of Ni surface alloys, can be measured and related to the chemical, catalytic, and electro-catalytic performance of these materials.

**Apr 1, 2009**  
**3:30 PM**  
**EB1, Rm 2018**

**Dr. Erik E. Santiso**  
Massachusetts Institute of Technology

***Modeling the nucleation of molecular crystals: order parameters and minimum free energy paths***

Crystallization is extensively used in the pharmaceutical and food industries, among others, to purify chemicals intended for human consumption. Many molecules, however, can crystallize into different polymorphs depending on the precipitation conditions (e.g. solvent, degree of supersaturation).

These polymorphs often exhibit different physical properties, which affects their suitability for various applications. For example, different polymorphs of a drug may have different dissolution profiles, and hence bioavailability, which makes the control of the crystallization process critical in drug manufacturing.

In this work, we combine a novel method to characterize the degree of order in molecular crystals with the string method in collective variables to obtain minimum free energy pathways for the nucleation of crystals from the melt and from aqueous solution. This approach will shed light on the mechanisms by which molecules come together and organize into crystalline structures, which is a first step in understanding polymorph selection. These results can be used to develop an improved, rational methodology for the manufacturing of drugs with a desired crystal structure.

**Apr 6, 2009**  
**10:45 AM**  
**1011 EB1**

**Dr. Navin Vardarajan**  
Massachusetts Institute of Technology

***Protease engineering: From molecular recognition to proteomics***

The exquisite selectivity and catalytic activity of natural enzymes have been shaped by the effects of positive and negative selection pressures during the long course of evolution. In contrast, in vitro engineering of novel enzyme variants capable of accepting new substrates typically results in a high degree of substrate promiscuity and lower catalytic turnover, compared to natural biocatalysts.

Using bacterial display and multiparameter flow cytometry, we have developed a novel methodology for emulating positive and negative selective pressures in vitro. Screening large combinatorial protein libraries with this technique has facilitated isolation of enzyme variants exhibiting high catalytic proficiency with novel, desired substrates, while simultaneously excluding those promiscuous variants with reactivity towards undesired analogs.

Having successfully demonstrated the feasibility of systematic engineering of protease specificity, we envisioned the application of engineered protease variants for the detection of post-translational modifications. Using multi-color flow cytometry, we have engineered OmpT variants that selectively cleave after post-translationally modified tyrosine (sulfo or 3-nitro), discriminating against both unmodified tyrosine and phosphotyrosine.

These results highlight the capacity for cutting edge protein engineering technologies to reshape how we approach solving practical, real world problems.



**Apr 13, 2009**  
**10:45 AM**  
**1011 EB1**

**Vibha Kalra**  
Cornell University

***Using External Fields to Control the Location of Nanoparticles in Block Copolymers: Experiments and Simulations***

Advances in materials synthesis and fabrication techniques allow an unprecedented control over the creation of novel building blocks such as polymers and particles. The first principle for effective utilization of these building blocks is to create techniques to control their assembly at length scales ranging from nanoscale to macroscopic scale.

In this seminar, I will talk about my research on fabrication of hierarchically structured materials that combine the functionalities of block copolymer nanocomposites with the advantages of nanofibers. One of the key findings of this work is that a much larger fraction of nanoparticles can be successfully placed (without agglomeration) within nanofibers compared to films of the same materials.

To zero in on the mechanism and to understand the thermodynamic and kinetic processes that drive nanoparticle placement in block copolymers during deformation, I will present my computational work using coarse grained molecular dynamics simulations. Here, I will talk about the effect of shear flow on different types of block copolymer/nanoparticle systems. Lastly, I will briefly discuss my ongoing work on effect of elongational flow on such systems.

**Apr 20, 2009**  
**10:45 AM**  
**EB1, Room 1011**

**Dr. Gengfeng Zheng**  
Northwestern University

***Developing New Functional Nanomaterials for Biosensing and Biophysical Studies***

Nanoscience and nanotechnology has attracted tremendous interest within the research community because new materials, structures and technologies could impact humankind in many significant ways.

My talk will focus on the synthesis of new nanomaterials along with structural and physical property characterization; fabrication of novel functional device structures; development of new methodologies for biophysical studies of interfacial properties between biomaterials and nanostructures; and ultrasensitive detection of chemical and biological species for clinical and bio-safety applications.

**Apr 20, 2009**  
**10:50 AM**  
**1011 EB1**

**Professor Michael C. Flickinger**  
Chemical & Biomolecular Engineering/Biotechnology Center

***What's so interesting About Microbial Paints and Inks?***

Reactive cells could play a significant role in the chemical industry as biocatalysts; for environmental remediation and energy generation if their reactivity could be significantly intensified and stabilized. One approach to intensification is to concentrate cells in thin coatings on surfaces.

Our group studies biocatalyst intensification and miniaturization (BIM) by developing approaches to concentrate cells in coatings combined with understanding non-growth gene expression to engineer highly reactive adhesive biocatalytic coatings. Model microbial systems studied by our group and collaborators include: high intensity oxidation of sugars and terpenes, stability and radiative light transfer modeling of a photo reactive biomimetic "leaf" generating H<sub>2</sub> from waste organics, gas-phase detection of volatile organics, and ink-jet inks for miniature biosensors, microfluidic or bioelectronic applications.

Future work by our group and collaborators will evaluate methods to generate adhesive monolayers of reactive cells and polymer particles.

**May 15, 2009**  
**11:00 AM**  
**EB1, Rm 2018**

**Dr. Krassimir Velikov**  
Unilever R&D, Netherlands

***Colloidal Delivery Systems for Micronutrients and Nutraceuticals***

The growing demand for functional foods promoting health and reducing the risk of diseases is largely driven by the increasing knowledge of the relationship between food ingredients and their impact on physiological functions and health. The delivery of functional ingredients, however, brings enormous challenges for the food industry; some of which are also encountered in pharmaceutical companies.

For example, the incorporation of micronutrients and nutraceuticals can compromise product functionality. The issues often encountered are related to solubility, taste, and stability of the functional ingredient or unwanted changes in the product stability, appearance, texture and taste.

The formulation of lyophobic bioactive molecules with high melting temperatures, can, as with many pharmaceutical drugs, also be problematic due to their limited solubility and bioaccessibility. To overcome these issues, novel approaches based on colloidal delivery systems have been developed.

In this talk, an approach based on the use of colloidal delivery systems in functional food design will be illustrated. The basic concepts for design and application of colloidal delivery systems will be exemplified. Finally, the differences from, and similarities to drug delivery issues will be discussed.