

Jan 7, 2013 10:40 AM Room 1011 - EB1	Peter Fedkiw Department of Chemical and Biomolecular Engineering – NCSU
<i>State of the Department</i>	

Jan 14, 2013 10:40 AM Room 1011 - EB1	Chuanbing Tang Department of Chemistry and Biochemistry - University of South Carolina
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Metallocene Polymers and Renewable Bio-based Polymers: Combining Functions and Architectures via Macromolecular Engineering

[Speaker's Website](#)

Macromolecular engineering allows the precision synthesis of structural details and complexities of macromolecules toward function-driven applications. This doctrine has been widely accepted across diverse fields of polymer science. We have adopted macromolecular engineering in conceptualizing, developing and expanding two research projects that are focused on central functional building blocks to design novel polymeric architectures. The first half of this presentation is about the introduction of cationic metallocene particularly 18-e cobaltocenium as a functional moiety into framework of ionic polyelectrolytes. The synthetic methodology encompasses from the derivatization of cobaltocenium monomers to controlled polymerization. Taking advantage of characteristic counter-ion dependent solubility, high structural stability and reversible redox chemistry of cobaltocenium, we have studied solution self-assembly of cobaltocenium-containing polyelectrolytes, and discovered new niche applications. The second half of this presentation will be focused on the development of renewable bio- based polymers from a class of hydrocarbon-rich biomass: natural resin acids. While synthesis of engineering polymers from simple thermoplastics to biodegradable block copolymers to biocomposites aim for sustainable materials, we will demonstrate how to utilize the unique structure and function of resin acids to develop a class of antimicrobial biomaterials.

References:

1. Ren L.; Hardy C. G.; Tang C. Synthesis and Solution Self-assembly of Side-Chain Cobaltocenium-containing Block Copolymers, *J. Am. Chem. Soc.*, 2010, 132, 8874-8875.
2. Ren L.; Zhang J.; Hardy C. G.; Ma S.; Tang C. Cobaltocenium-containing Block Copolymers: Ring-opening Metathesis Polymerization, Self-assembly and Template Synthesis of Inorganic Nanoparticles. *Macromol. Rapid Commun.*, 2012, 33, 510-516.
3. Yao K.; Wang J.; Zhang W.; Lee J. S.; Wang C.; Chu F.; He X.; Tang C. Degradable Rosin-Ester- Caprolactone Graft Copolymers, *Biomacromolecules*, 2011, 12, 2171-2177.
4. Wang J.; Chen Y.; Yao K.; Wilbon P.; Zhang W.; Ren L.; Zhou J.; Nagarkatti M.; Wang C.; Chu F.; He X.; Decho, A. W.; Tang C. Robust Antimicrobial Compounds and Polymers derived from Resin Acids. *Chem. Commun.*, 2012, 48, 916-918.

Jan 22, 2013
10:40 AM
BTEC - Room 135

Ryan Lively
School of Chemical and Biomolecular Engineering - Georgia Tech

Enabling advanced biofuel production through materials-inspired energy efficient separations

[Speaker's Website](#)

As corn-based biofuels reach their practical limits, advanced algae-based biofuels are poised to supply the rapidly increasing demand for renewable fuels. Large energy costs in biorefineries using traditional separation techniques for dilute feedstocks are currently a hurdle, but also a major opportunity for innovation. Advanced materials and their manufacturing into low-cost, energy-efficient separation devices to meet this challenge will be the focus of the talk. First, post-combustion CO₂ capture will be discussed as an economical carbon source for the algae. A highly scalable materials production technique—fiber spinning—is used to create high-flux polyimide hollow fiber membranes as well as multi-layer hollow fiber sorbents that function as integrated adsorbing heat exchanging devices. Flexible zeolitic imidazolate frameworks (ZIFs) are identified as promising candidates for advanced filler materials in polymer-inorganic hybrids. The versatility of the fiber sorbent platform is illustrated. Materials synthesis, bench-scale module testing and techno-economic analysis of these fiber-based systems will be presented. Besides the CO₂ capture challenge, purification of dilute ethanol feeds must be addressed. In this regard, a highly hydrophobic zeolite is a uniquely attractive candidate for dilute ethanol recovery. Fundamental transport and thermodynamic characterizations of a suitable zeolite for this application are presented. Exceptionally high ethanol/water selectivities are obtained for the neat zeolite. Zeolite morphology control is demonstrated, as is the inclusion of high aspect ratio forms of the zeolite into hybrid materials. Routes forward for both separations are discussed.

Feb 4, 2013
10:40 AM
Room 1011 - EB1

Baron Peters
Department of Chemical Engineering - UC Santa Barbara

Solute Precipitate Nucleation: Mechanistic Insight from Theory and Simulation

[Speaker's Website](#)

Nucleation is the process that creates the first stable embryo of a new phase to initiate a phase transition. Even for simple single component systems, nucleation processes with long induction times pose serious challenges for molecular simulation. The difficulties are even more acute for multi-component condensed phase nucleation processes where most applications lie. Our recent advances in this latter area show how the thermodynamics and dynamics of nucleation, including structural polymorphism, can be understood using a combination of simulation and theoretical analysis.[1,2] Applications to methane hydrate nucleation and polymorph selection in glycine nucleation will be presented.[3,4] Finally, I will

discuss evolving efforts to understand how mass transfer effects can alter predictions of the classical theory.[5]

- [1] Peters, J. Chem. Phys. 131, 224103 (2009)
- [2] Duff, Peters, J. Chem. Phys. 135, 134101 (2011)
- [3] Knott et al. J. Am. Chem. Soc. (2012)
- [4] Duff, Peters, in preparation
- [5] Peters, J. Chem. Phys. 135, 044107 (2011)

Feb 11, 2013

10:40 AM

Room 1011 - EB1

Isaac Sanchez

Department of Chemical Engineering - University of Texas at Austin

Computational Modeling of the Void Structure in Polymeric Glasses and Globular Proteins

[Speaker's Website](#)

Within a polymer thin film, free-volume elements have a wide range of size and topology. This broad range of free-volume element sizes determines the ability for a polymer to perform molecular separations. Using atomistic models, cavity size (free volume) distributions were determined by a combination of molecular dynamics (MD) and Monte Carlo methods for 6 thermally rearranged (TR) polyimides and their precursors. Diffusion, solubility, and permeation of gases in TR polymers and their precursors were simulated at 308 K, with results that agree with experimental data.

A similar methodology has been used to characterize the void structure within globular proteins. The method produces a spectrum of the empty cavities and channels within a protein and has been labeled "computational spectroscopy." Molecular dynamics provides a picture of structural changes with time. Since water molecules can occupy the void spaces, the MD simulation also reveals how water can move in out of a protein. Water channels also provide pathways for the migration of small molecules such as oxygen to the active site within the protein. Application to myoglobin and some of its mutants will be used to illustrate the methodology and its potential for drug design.

Feb 12, 2013
10:40 AM
Room 135 BTEC

Haiqing Lin
Membrane Technology and Research, Inc

Molecular Engineering of Polymeric Membrane Materials for H₂ Purification and CO₂ Capture

Growing evidence indicates that the CO₂ emissions from the combustion of fossil fuels are contributing to global climate change. One approach to controlling CO₂ emissions to the atmosphere is carbon capture, utilization and sequestration (CCUS) from large point sources, such as H₂ and power plants. Pre combustion capture from syngas has been considered as an economically viable route. In this scheme, gasification of fossil fuels produces syngas, which is further converted to CO₂ and H₂. The CO₂ must be removed and captured prior to H₂ utilization for refinery hydrogenation reactions or combustion in the power plant turbines. Membrane technology is an attractive approach to H₂ purification and CO₂ capture because of inherent advantages such as high energy efficiency. This presentation will systematically examine the need of membrane technology as a low cost and energy efficient separation technology enabling the CCUS via pre combustion route. I will discuss how we rationally design polymeric membrane materials to achieve the combination of high CO₂ permeability and high CO₂/H₂ selectivity. More specifically, this talk will discuss the molecular engineering of poly(ethylene oxide) (PEO) containing polymers for improvement in mixed-gas CO₂/H₂ separation performance. Interestingly, these materials exhibit unconventional increase in mixed gas CO₂/H₂ selectivity as CO₂ feed partial pressure increases. The structure and property correlation in these PEO containing polymers will also be interpreted using a modified free volume model.

Feb 18, 2013

10:40 AM

Room 1011 - EB1

Stefano Menegatti

Department of Chemical and Biomolecular Engineering – NCSU

Next generation peptide ligands for bioseparations, diagnostics, and biological research

The search for novel affinity ligands with high selectivity for biomolecules is a common thread that unites research efforts in biomedicine and biotechnology, from the development of downstream processes for biotherapeutics to the design of novel diagnostic agents and drugs. Currently, protein ligands and antibodies play a key role in these fields, owing to their high affinity and selectivity for target biomolecules. On the other hand, they suffer from high production costs, and low chemical and biochemical stability. Small peptide ligands represent a valid alternative to protein ligands. While they can be comparable to proteins in terms of target affinity and selectivity, peptides can be produced synthetically in large amounts, thus reducing costs.

The research described in this presentation combines the recent advancement in peptide synthesis, bioconjugation techniques, and modeling tools for simulating protein-peptide interactions to develop peptide ligands amenable to large scale purification of biotherapeutics as well as diagnostic and therapeutic applications. This presentation will focus on the development of novel peptide-based technologies that hold great promise for bioseparations and medicine: 1) the development of adsorbents based on linear peptide ligands with binding capacity and chemical stability comparable to those of the most advanced affinity media; 2) the use of non-natural amino acids to develop protease-resistant peptide ligands for purifying proteins from animal plasma; 3) the design and screening of innovative biological (mRNA-display) and synthetic (solid-phase) libraries of cyclic peptides to identify highly selective affinity ligands for the purification of antibodies; and 4) the use of modified cyclic peptides for the site-selective labeling of antibodies for diagnostic or therapeutic applications. In closing, some potential new directions for this work and their implications will be discussed.

Feb 25, 2013

10:40 AM

Room 1011 - EB1

Giorgio Carta

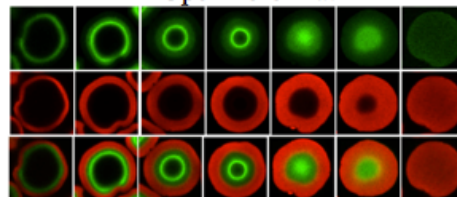
Department of Chemical Engineering - University of Virginia

Transport Phenomena in New and Improved Stationary Phases for Downstream Processing of Biopharmaceuticals

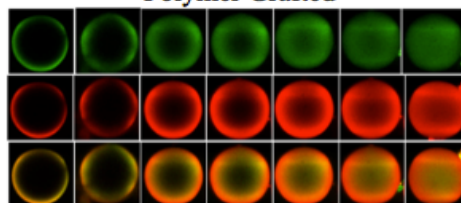
[Speaker's Website](#)

Downstream processing of pharmaceutical proteins such as monoclonal antibodies (mAbs) is currently limited by capacity and rate bottlenecks. Binding capacity is limited by the large size of these biomolecules while their slow diffusion requires long processing times. The key to removing these bottlenecks is thus to devise new and improved stationary phases for protein chromatography where both capacity and mass transfer rates are increased without sacrificing mechanical strength so that more can be adsorbed faster. Composite materials, incorporating soft, charged polymers supported by a rigid structure have been introduced for this purpose in recent years and appear to be a significant step in the desired direction. But how do these materials achieve faster transport without comprising capacity? The combined use of macroscopic measurements, microscopic measurements using confocal laser scanning microscopy to track the movement of proteins within the chromatographic particles, and transport modeling provides mechanistic insight. We show that protein capacity is increased by multilayer binding while transport is enhanced by closerange biomolecular interactions within the charged polymers giving rise to a large diffusional driving force. We also address the large effects that subtle charge variants arising from post-translational modifications have on chromatography and transport in these materials. Mechanistic models and conditions under which these composite matrices show promise for various applications are illustrated and an outlook for the future is provided.

Open Pore Matrix



Polymer Grafted



Mar 18, 2013
10:40 AM
Room 1011 - EB1

Tim Fornes
Lord Corporation

Managing Heat, Electricity, and Lightning Through Understanding of (Nano)composite Structure-Property Relationships

Polymer composites, especially as those derived from fillers, continue to be a subject of intense research and development in both academia and industry. A common goal in this field is to achieve very efficient property enhancements through chemical and/or mechanical manipulation of the dispersed filler phase. Unfortunately, many approaches, including those involving nanofillers, still lead to undesirable sacrifices properties such as strength, toughness, adhesion, and/or viscosity. Recent developments at LORD Corporation have shown that property tradeoffs can be greatly minimized by developing a thorough understanding of the relationships between chemical structure, physical structure, and composite properties. This presentation will highlight some examples of how such structure-property knowledge was used to create novel materials needed for commercial applications such as thermal interface materials, electromagnetic shielding, and lightning strike protection coatings for composites.

Mar 25, 2013
10:40 AM
Room 1011 - EB1

Ram B. Gupta
Program Director - Energy for Sustainability -
National Science Foundation

Energy for Sustainability

Today's world is facing two critical challenges: (1) high fuel prices, and (2) climatic changes. Both of these are linked to the overdependence on the fossil fuels: petroleum, natural gas, and coal. The transport is almost totally dependent on fossil particularly petroleum based fuels such as gasoline, diesel fuel, liquefied petroleum gas, and natural gas. The combination of rising oil prices, issues of security, climate instability and pollution, and deepening poverty in rural and agricultural areas, is propelling governments to enact powerful incentives for the use of renewable energy.

In this talk, NSF's Energy for Sustainability program will be presented. This program supports fundamental research and education that will enable innovative processes for the sustainable production of electricity and transportation fuels. Processes for sustainable energy production must be environmentally benign, reduce greenhouse gas emission, and utilize renewable resources. Projects include those related to biofuels, photovoltaic solar energy, wind energy, and advanced batteries for transportation.

Apr 1, 2013
10:40 AM
Room 1011 - EB1

Ruben Carbonell, Robert Kelly and Bala Rao, Moderator - Carol Hall

Roadmap to Success in Grad School: a Faculty Panel

What steps should you be taking to maximize your success as a graduate researcher? Three faculty, Ruben Carbonell, Robert Kelly and Bala Rao, give their take on, and answer questions about, how to get where you want to go in graduate school, and the expectations that faculty have but don't always spell out. The moderator is Carol Hall. Please prepare questions in advance and submit them to Professor Hall by e-mail.

Apr 15, 2013
10:40 AM
James B. Hunt Jr. Library

Robert Langer
Department of Chemical Engineering – MIT

McCabe Lecture - Biomaterials and biotechnology: From the discovery of the first angiogenesis inhibitors to the development of controlled drug delivery systems and the foundation of tissue engineering

[Speaker's Website](#)

Advanced drug delivery systems are having an enormous impact on human health. We start by discussing our early research on developing the first controlled release systems for macromolecules and the isolation of angiogenesis inhibitors and how these led to numerous new therapies. For example, new drug delivery technologies including nanoparticles and nanotechnology are now being studied for use treating cancer and other illnesses. We then discuss ways of developing novel microchips for drug delivery. Approaches for creating new biomaterials are then evaluated and examples where such materials are used in brain cancer and shape memory applications are discussed. Finally, by combining mammalian cells, including stem cells, with synthetic polymers, new approaches for engineering tissues are being developed that may someday help in various disease. Examples in the areas of cartilage, skin, blood vessels and spinal cord repair are discussed.

Apr 19, 2013
2:30 PM
Room 119 BTEC

Giovanni Ciccotti
Dipartimento di Fisica, Universita di Roma, La Sapienza/School of Physics,
University College of Dublin

Time-dependent Non-equilibrium Molecular Dynamics

We present a way to extend stationary state (equilibrium and nonequilibrium) Molecular Dynamics to time dependent nonequilibrium situations, including the dynamical processes of response and relaxation. The procedure, which we have called Dynamical Non-Equilibrium Molecular Dynamics (D-NEMD), to distinguish it from standard NEMD, only used to simulate stationary nonequilibrium states, is based on a generalization of linear response theory. The idea has been formulated by Onsager in the thirties in metaphysical language; given a solid foundation in the fifties by Green and Kubo (in the linear and nonlinear regime); and adapted

to MD simulations by the present author (in collaboration with G.Jacucci and I.R.Mac Donald) in the seventies. It has been called the nonlinear Kubo-Onsager relation, connecting dynamical nonequilibrium averages or dynamical relaxations to stationary probability distribution functions (initial distribution) suitably sampled. To show the power of the method we apply it to the study of the hydrodynamic relaxation of an interface between two immiscible liquids.

Apr 22, 2013

10:40 AM

Room 1011 - EB1

Paulette Clancy

School of Chemical and Biomolecular Engineering - Cornell University

Covalent Organic Frameworks as Prototypical Ordered Heterojunction for Solar Cells

[Website](#)

There is growing momentum behind the use of computational tools to go beyond their traditional role to provide mechanistic information and move into the realm of a predictive experiment-guiding mode. Simulations are poised to help guide the selection of candidate materials and the design of heterojunctions for electronic devices. While bulk heterojunctions are currently the norm for heterojunction design for all-organic solar cells, it would be more desirable to have a self-assembly process that forms ordered heterojunctions into a relatively rigid structure featuring electron- and hole- directing "superhighways" that can lead to efficient charge separation.

We will present one such family of ordered heterojunctions, featuring a new class of materials called Covalent Organic Frameworks, and look at the use of molecular-scale computations to study the self-assembly (stacking) of these moieties and the implications for the construction of COF-fullerene "p-n" junctions. We will discuss two-dimensional covalent organic frameworks (2D COFs) that are constructed from boron-containing, "connectors" and hydrocarbon "linkers," evaluated using a combination of multiscale modeling techniques from Molecular Mechanics to Density Functional Theory (DFT) calculations.

None of these 2D COFs stack in the exact eclipsed "a-a" configuration assumed originally to be likely for these materials. Instead, adjacent layers adopt small offsets (1.4-2.5 Å) for 33 COF candidates in this class. These offset values are determined by a combination of attractive dispersion and repulsive electrostatic interaction energies, which give rise to a series of distinctive patterns in the Potential Energy Surfaces (PES). Symmetry in the PES creates a random stacking of COF layers, precluding the formation of stacking patterns with long-range order, such as postulated staircase, helical, or zigzag arrangements. Although these offsets are often small relative to the size of the COF unit cell, we show that they are sufficient to impede the filling of COF pores with large "guests," such as fullerenes. Finally, we use a combination of topology and chemical composition to provide a simple correlation that will allow researchers to predict inter-layer offsets and interaction energies without performing any molecular simulations. Uncovering such design principles should pave the way to target the creation of COFs with prescribed properties.

Apr 24, 2013

3:00 PM

Room 315 Riddick

Labs, North Campus

Giovanni Ciccotti

Dipartimento di Fisica, Università di Roma, La Sapienza/School of Physics, University College of Dublin

Challenges for Molecular Dynamics Simulations

Molecular Dynamics simulations (MD), born in 1957, have now a long history of successes, essentially based on the realization of the Boltzmann program to explain the properties of macroscopic matter (essentially in equilibrium) on the basis of (classical) atomistic statistical mechanics. In the years MD has evolved from the simulation of simple (point particles), small systems, sufficient to derive the thermodynamic properties of simple phases, to that of (i) large, almost macroscopic, systems and (ii) complex aggregates of (macro-)molecules. These developments have had a profound impact on biochemistry and, more generally, biophysics. In the other direction, the atomistic simulations of simple (point particles) but large systems have brought MD from thermodynamics to hydrodynamics and beyond. These are, at present, its major challenges. In the present talk I

- i. describe the essential content of standard MD simulations and
- ii. show how it can be generalized to cover
 - a. complex simulations of macro-/bio-molecules or
 - b. reconstruction of complex hydro-dynamical behavior.

The presentation will cover both the theoretical treatments and a few pleasant illustrative applications.