Jan 11, 2016
10:40 AM
Room 1011, EB1

Dr. Athanassios Panagiotopoulos
Princeton University

Molecular Simulation of Phase Equilibria: Progress and Challenges

Gubbins Lecture

A major topic in chemical engineering thermodynamics is the calculation of the phase behavior of pure components and mixtures from molecular-based information. The Gibbs ensemble and grand canonical Monte Carlo methods enable the calculation of phase diagrams for fluids composed of complex, realistic potentials. For solid phases and for determination of activity coefficients and solubilities in electrolyte solutions, thermodynamic integration methods provide a direct path to the phase behavior and thermodynamic properties. Alternatively, open-source fast and scalable molecular dynamics codes have been developed that can be used in two-phase simulations of phase equilibria. The main remaining challenges in this area are related to the inadequacies of the current generation of force fields, which lack important physical features such as polarizability. Work in this area has been deeply influenced by the seminal contributions of Prof. Gubbins over the past several decades.

Jan 12, 2016
3:30 PM
Room 135, BTEC

Dr. Athanassios Panagiotopoulos
Princeton University

Self-Assembly in Nanoparticle and Polymer Systems

Gubbins Lecture

This lecture focuses on simulations of pattern formation in block copolymer thin films, as well as colloid-polymer systems. For the block copolymer systems, we utilize a recently developed theoretically informed coarse graining model that preserves chain connectivity, microphase separation and finite compressibility of the melt. Our simulations show that static films have morphologies highly sensitive to film thickness and wall interactions, and that shear can be employed to induce long-range ordering. For colloid-polymer systems, we find that void topology differences between “nearby” crystal structures (e.g., face-centered cubic and hexagonal closed packed) can be used to direct crystallization towards desired polymorphs. Under flow, colloids migrate to the centerline of micro channels, expelling the polymer chains to the sides. This behavior was recently identified in experiments, and may be exploited to separate and capture particles at the sub-micrometer scale using simple microfluidic devices.

Jan 19, 2016
10:40 PM
Room 135, BTEC

Dr. Burcu Gurkan
University of Akron

Absorptive and Electrochemical CO2 Separation Processes

Among the grand challenges that engineers face today is the global climate change. Lessons learned from the industrialization era; 21st century engineers seek alternative approaches and processes that are environmentally benign. To mitigate global climate change and aid in efforts to reduce CO_2 emissions from major contributors, specifically coal-fired power plants, discovery of novel materials and processes are essential for the foreseeable future. The long-term solution to this problem requires the development of carbon-neutral energy infrastructure; one that demands significant improvements in the current energy storage devices to make this effort viable and economical. In particular, the next generation batteries demand breakthroughs in energy and power density, electrode design and electrolytes. In this talk, Dr Gurkan will present her past and ongoing research addressing the (i) design of novel solvents for absorptive CO_2 capture, (ii) electrochemically mediated separation of CO_2, and (iii) functionalized ordered mesoporous carbon for sodium-ion battery electrodes.

Jan 27, 2016
10:20PM
Room 135, BTEC

Dr. Kelsey Hatzell
Lawrence Berkley National Lab

Conducting (flowable) Suspension Electrodes for Water and Energy Applications

Suspension or semi-solid electrodes have recently gained increased attention for large-scale applications such as grid energy storage, capacitive water deionization, and wastewater treatment. A suspension electrode is a multiphase material system comprised of an active (charge storing) material suspended in an ionic solution (electrolyte). Gravimetrically, the electrolyte is the majority component and aids in the physical transport of the active material. This principle enables, for the first time, scalability of electrochemical energy storage devices (supercapacitors and batteries) previously limited to small and medium scale applications. This talk will combine classical aspects of electrochemistry, colloidal science, material science, fluid mechanics and rheology to describe ion and charge percolation, adsorption of ions, and redox charge storage processes in suspension electrodes. Moreover, novel techniques for examining a flow-electrodes 'microstructure' will be introduced. Finally a discussion of primary challenges and future research directions will be included.

Feb 1, 2016
10:40 AM
Room 1011, EB1

Dr. Blair Brettman
University of Chicago

Molecular Engineering for Integrated Product Development

Traditionally the innovation process for new products proceeds linearly through three stages: discovery, development and scale-up to launch. While this can be successful in many cases, failure in the scale-up phase is common and costly, particularly in pharmaceutical product development when an average of $430 million is spent on research per drug prior to human trials. The likelihood of successful transition to scale-up and launch can be increased by employing an integrated approach to innovation, where the effects on molecular level behavior of manufacturing processes and the highly complex mixtures used for scaled-up products are considered throughout the discovery and development phases. As part of a center dedicated to transitioning pharmaceutical manufacturing from batch to continuous processes, I focused on developing a downstream processing technology, electrospinning, to be useful for producing a wide variety of pharmaceutical products, including those containing crystalline and amorphous drug forms. With an integrated innovation approach, molecular level behavior of the drug and polymer characterized by solid state NMR was tied to the end product properties as well as influences from the manufacturing process. This enabled the development of a process to produce electrospun products containing crystalline drugs as well as provided confidence for producing stable amorphous drug forms. Based on this detailed understanding of the product and process, electrospinning was selected as one of the technologies to incorporate into the start-up that formed from the center, Continuus Pharmaceuticals.

Feb 5, 2016
10:40 AM
Room 1007, EB1

Dr. Lauren Zarzar
Massachusetts Institute of Technology

Dynamic Soft Materials: Gels, Bubbles, and Drops

Dynamic materials that sense and adapt to their surroundings are primed to be integral components of future technologies. However, designing dynamic behavior into what is perhaps an otherwise static material is a significant challenge that often requires development of novel chemo-mechanical transduction strategies. We will explore different approaches by which chemical or environmental stimuli can be coupled to movement within nano/microscale materials in order to create systems with uniquely responsive and functional behavior. Three such soft materials will be highlighted: 1) hydrogel-driven actuators, 2) micro-environments enabling bubble-directed flow, and 3) reconfigurable complex droplets.

Feb 10, 2016
10:20 PM
Room 135, BTEC

Dr. Milad Abolhasani
Massachusetts Institute of Technology

Microscale Multi-Phase Flow Technologies for Sustainability, Pharmaceutical Chemistry, and Nanomaterial Synthesis

Molecular transport spanning multiple phases and drastically different length scales occurs in our daily life and controls our health and surrounding environment; such transport phenomena include greenhouse gas generation from combustion of fossil fuels and drug transport and delivery within the human body. A fundamental understanding of the microscale transport mechanisms would facilitate the development of energy-efficient carbon capture technologies, the design of more effective drug formulations, and the synthesis of environmentally friendly nanomaterials. Capitalizing on the well-defined interfacial area and enhanced mass and heat transfer rates enabled by flow segmentation, microscale multi-phase flow platforms can be exploited for fundamental and applied studies of single/multi-phase chemical reactions as well as for tuning and optimization of physico-chemical properties of nanomaterials.

This seminar will focus on microscale technologies tailored for studies of transport mechanisms in multi-phase flow. First, a continuous microfluidic strategy for systematic examination of microscale gas-liquid transport phenomena through automated screening of carbon dioxide (CO_2) mass transfer and solubility in different physical/chemical absorbents will be discussed. Next, adaptation of this continuous microscale strategy for measurement of the thermodynamic characteristics of gas-liquid reactions and CO_2-triggered liquid-liquid phase separation process will be presented. Finally, the mass transfer characteristics of a recently developed multi-phase oscillatory flow strategy for *in-situ* studies of relatively long (10-60 min) physical/chemical processes in a small (200 uL) flow reactor will be discussed. Case studies will include palladium-catalyzed C-C and C-N coupling reactions, octanol-water partitioning of drug molecules, and solution-phase processing of semiconductor nanocrystals.

Feb 22, 2016
10:40 AM
Room 1011, EB1

Dr. Lilian Hsao
Massachusetts Institute of Technology

Engineering Soft Matter Through Particle Shape and Surface Features

A central challenge in soft matter and materials science is the microscopic engineering of functional materials. Incorporating anisotropy here is of general interest, for example in actin networks, clay platelets, and polymer nanocomposites where geometry, ordering, and kinetics all play important roles in determining their properties. Nevertheless, forming a general connection between microstructure and macroscale properties is not trivial. Here, I focus on the self-assembly and mechanics of colloidal materials with an emphasis on how shape anisotropy and interaction potential can be used to guide their design. I will first discuss the relevance of the physical interactions that give rise to a general class of colloidal gels. Then, I will introduce structural rigidity in the context of gels undergoing large deformations, and how shape anisotropy can introduce unusual states through kinetic trapping. Lastly, I will show that the slowed rotational dynamics caused by surface roughness can lead to enhanced shear thickening that is not seen with smooth colloids. These results collectively show that particle-level interactions provide a powerful means to design soft materials at multiple length scales.

Feb 24, 2016
10:20 AM
Room 135, BTEC

Dr. Mary Elting
University of California, San Francisco

Mechanics of Cell Division: Building Biological Machinery from Molecular-scale Parts

In contrast to many large-scale mechanical structures, such as the bridges or skyscrapers that we build, biological structures must allow dynamics and turnover of their constituent parts while retaining their mechanical integrity. What are the underlying principles for building such structures? Here, I focus on the mitotic spindle, the microtubule machine that delivers chromosomes to two daughter cells during cell division. The accuracy and robustness of its function are essential to health. While we have identified many of the molecules essential to spindle function, we do not understand how larger scale mechanical properties emerge. In part, this is because of the difficulty of exerting controlled mechanical perturbations inside live cells. By combining laser ablation, quantitative analysis, and molecular perturbations, I first ask how chromosome-bound microtubules anchor to the mammalian spindle, and find that the spindle anchors them redundantly and highly locally. Second, I ask how the spindle robustly maintains microtubule attachment, despite dynamic forces from in and outside the cell, and find that it does so by rapidly detecting and repairing breaks in attachment. In my own lab, I will re-engineer molecular-scale spindle building blocks to rewire self-assembled microtubule structures in vitro and in vivo and probe how mechanical properties of higher order structures emerge across scales.

Feb 26, 2016
10:40 AM
Room 1007, EB1

Dr. Maryam Peer
Massachusetts Institute of Technology

Polymer-derived Carbon-based Materials with Tailored Properties: Design and Application

Porous materials are the key component in many industrial applications including catalysis, separation, adsorption and energy conversion. Particularly, the depletion of fossil fuels and increasing interest in renewable energy sources call for materials with tunable and desired characteristics. The efficiency of porous materials is mainly dictated by their textural and morphological properties along with the chemical composition. Polymer-derived porous carbon materials are promising candidates as they offer advantages such as high thermal and chemical stability, large surface area and inert surface chemistry prone to functionalization. Despite the intensive research in this field, the design and development of carbon-based materials with desired porous network, geometry and functionality via a simple one-step synthesis approach, remains a challenge. Soft-templating technique coupled with the right choice of monomers and synthesis conditions, serve as a powerful platform for synthesizing carbon nanostructures with tuned pore size, morphology and catalytic activity. In this talk I will present my past and current research on i) polymer-derived carbon-based shape selective catalysts, and ii) high surface area nitrogen-doped porous carbons with enhanced visible light absorption. I will also briefly discuss the key findings of my recent study on continuous reactions in microfluidic reactors for safe and green production of pharmaceutical intermediates.

Mar 8, 2016
4:30 PM
Room 135, BTEC

Dr. Nicholas Abbott
University of Wisconsin-Madison

Topological Defects in Liquid Crystals as Templates for Molecular Self-Assembly

MRSEC Seminar Series

Topological defects in liquid crystals (LCs) have been widely used to organize colloidal dispersions and template polymerizations, leading to a range of elastomers and gels with complex mechanical and optical properties. However, little is understood about molecular-level assembly processes within defects. This presentation will describe an experimental study that reveals that nanoscopic environments defined by LC topological defects can selectively trigger processes of molecular self-assembly. By using fluorescence microscopy, cryogenic transmission electron microscopy and super-resolution optical microscopy, key signatures of molecular self-assembly of amphiphilic molecules in topological defects are observed - including cooperativity, reversibility, and controlled growth of the molecular assemblies. By using polymerizable amphiphiles, we also demonstrate preservation of molecular assemblies templated by defects, including nanoscopic “o-rings” synthesized from “Saturn-ring” disclinations. Our results reveal that topological defects in LCs are a versatile class of three-dimensional, dynamic and reconfigurable templates that can direct processes of molecular self-assembly in a manner that is strongly analogous to other classes of macromolecular templates (e.g., polymer—surfactant complexes). Opportunities for the design of exquisitely responsive soft materials will be discussed using bacterial endotoxin as an example.

Mar 14, 2016 10:40 AM Room 1011, EB1	**Dr. Ronghui Wang** University of Arkansas

Innovative Biosensors for Rapid Detection of Pathogenic Bacteria and Viruses in Agriculture and Food

Monitoring animal and plant diseases and detecting foodborne pathogenic bacteria and viruses are critical for sustainable agricultural and food systems around the world. Advanced technology is needed for effective detection of these pathogens to minimize the economic loss and improve human health. Biosensors, which combine a target-specific biological element with a transducer and signal processing unit, offer the most promising solutions and address some of the modern-day needs for rapid and sensitive detection of pathogens in real time. In this presentation, the development of several types of innovative biosensors are reported for rapid, sensitive, and specific detection of pathogenic bacteria and viruses in agriculture and food. A TiO_2nanowire bundle microelectrode based immunosensor was developed and demonstrated for more sensitive and rapid detection of *Listeria monocytogenes*, one of the major foodborne pathogens. It was based on the combination of an impedance biosensor with highly sensitive semiconductive nanomaterial microelectrodes modified with specific capture antibodies. The detection limit was 103 times lower than the conventional Dot-Blot analysis. As a representative of pathogenic viruses in agriculture, high-pathogenicity avian influenza virus (AIV) H5N1 was detected using a novel bio-nanogate based biosensor. An aptamer-based bifunctional bio-nanogate was designed and tested, which could selectively respond to target pathogens and control enzymatic reaction for electrochemical measurements. It was successfully applied for sensitive, selective, rapid, and label-free detection of AIV H5N1. It is entirely possible that the same biosensor technology could also be used for rapid and sensitive detection of pathogenic bacteria and viruses from plants.

Mar 16, 2016 10:20 AM Room 135, BTEC	**Dr. Qingshan Wei** UCLA

Translating Biophotonics from the Lab to the Point of Care

The past decade has witnessed the rapid advance of optical imaging in **s**patial resolution, **s**ensitivity, **s**pecificity, and **s**peed. The fifth “S”, smart imaging system, is newly emerging and greatly transforming the biophotonics and biomedical tests from the lab to the point of care. My talk will first introduce a new strategy to improve imaging sensitivity by the development of a universal image contrast enhancement mechanism named dynamic contrast. I will showcase two examples of dynamic contrast that is introduced by magnetic and photothermal modulation, respectively. The second part of my talk will highlight my recent research in creating smart imaging, sensing, and diagnostic tools based on mobile phones, and their applications for molecular detection such as single DNA molecule imaging, KRAS mutation detection, digital LAMP/ELISA assay, and clinical vaccination testing. Promising future directions of sensitive yet portable imaging and sensing technologies towards precision medicine, global health, and plant diseases will also be discussed.

Mar 21, 2016 10:40 AM Room 1011, EB1	**Dr. Gregory Voth** University of Chicago

Theory and Simulation of Biomolecular Systems: The Multiscale Challenge

A multiscale theoretical and computational methodology will be discussed for studying biomolecular systems across multiple length and time scales. The approach provides a systematic connection between all-atom molecular dynamics, coarse-grained modeling, and mesoscopic phenomena. At the heart of the approach is a method for deriving coarse-grained models from protein structures and their underlying molecular-scale interactions. This particular aspect of the work has strong connections to the theory of renormalization, but it is more broadly developed and implemented for heterogeneous biomolecular systems. A critical component of the methodology is also its connection to experimental structural data such as cryo-EM or x-ray, thus making it “hybrid” in its character. Applications of our multiscale simulation approach to elaborate key features of complex processes such as the HIV virus capsid assembly and ATP hydrolysis driven actin filament dynamics will be presented as time allows.

Mar 28, 2016
10:40 AM
Room 1011, EB1

Dr. Wei Gao
NCSU

Graphene Oxide in Supercapacitors and Fuel Cells

Graphite oxide (or graphene oxide, GO), which was once noted as an important precursor to graphene(*1*), has been established as an important and technologically relevant material in the last five years. There now exists an extensive literature regarding the synthesis, chemical structure, reactivity, properties of GO, as well as its use in multiple applications. However, GO has recently been reported to degrade after about a month at room temperature(*2*). Loss of epoxy groups is believed to be the major structural change during the degradation process of GO. This structural change presents a significant challenge for all potential applications of GO. In my presentation, I will discuss our work using films of GO as a proton conductor in both supercapacitors(*3*) and hydrogen-air fuel cells(*4*) and how its properties may change over time. I will also show that degraded GO can regain epoxy groups with ozone treatment as indicated by solid-state 13C NMR, and FTIR analysis. The measured proton conductivity of ozone treated GO (OGO) is 75% higher than that of GO aged for more than a month in solution. Overall, free-standing OGO films offer improved device performance when used in supercapacitors and hydrogen fuel cells as proton conductors.

1. **W. Gao, L. B. Alemany, L. Ci, P. M. Ajayan, New insights into the structure and reduction of graphite oxide. *Nature Chemistry* 1, 403 (2009).**

2. **S. Kim *et al.*, Room-temperature metastability of multilayer graphene oxide films. *Nature materials* 11, 544 (2012).**

3. **W. Gao *et al.*, Direct laser writing of micro-supercapacitors on hydrated graphite oxide films. *Nature Nanotechnology* 6, 496 (2011).**

4. **W. Gao *et al.*, Ozonated Graphene Oxide Film as a Proton-Exchange Membrane. *Angewandte Chemie International Edition* 53, 3588 (2014).**

Apr 4, 2016
10:40 AM
Room 1011, EB1

Dr. Amy Karlsson
University of Maryland, College Park

Engineered Proteins and Peptides as Versatile Biological Tools

Our lab uses rational design and directed evolution to engineer proteins and peptides as molecular tools for studying protein-protein interactions and for designing better therapeutics. One thrust of our work is developing improved approaches for assays involving antibody fragments. We have developed a simple and robust method to immobilize antibody fragments that allows us to efficiently immobilize antibody fragments without purification. Another thrust of our work is engineering peptides for targeting the pathogen *Candida albicans.* We are engineering antifungal peptides for reduced protease susceptibility and are harnessing peptides as molecular vehicles for delivering cargo into the cytosol of *C. albicans*. A third thrust of our work is engineering antibody fragments that fold and function inside cells, where the reducing environment typically prevents antibodies from properly folding and functioning. We isolated an antibody fragment that binds to the apoptosis inhibitor survivin and are evolving this antibody to allow its use in knocking down the function of survivin in cancer cells. The protein engineering strategies we use and develop in our lab will enable new applications of proteins and peptides in studying biological phenomena and new approaches to therapeutic development.

Apr 14, 2016 4:30 PM Room 135, BTEC	**Dr. Eric Weeks** Emory University

Flow of Amorphous Solids Modeled with Emulsion Droplets

MRSEC Seminar Series

We use quasi-two-dimensional emulsions as experimental models to study the flow of jammed materials (amorphous solids). Our emulsions are oil droplets in water and are compressed between two parallel glass plates so that the droplets are deformed into pancake-like disks. We use microscopy to observe these droplets as they flow. From the deformed outlines of the droplets, we can measure all of the inter-droplet forces to within 10%. In this way, we study the relationship between the local stresses in the system and the rearrangements as the sample is sheared. In particular, we find that at very slow flow rates (quasi-static flow), we see large avalanches of rearrangements, whereas at higher flow rates rearrangement events occur more frequently but involve fewer droplets. The simplest rearrangement involves four droplets (a 'T1 event') and we confirm theoretical predictions for the quadrupolar spatial pattern of the stress redistribution around the T1 events.

Apr 18, 2016 10:40 AM Room 1011, EB1	**Dr. Nilay Chakraborty** University of Michigan - Dearborn

Engineering Cells for Biostability

The ability to preserve cells and tissue components for long term is of great clinical importance for successful implementation of multitude of cutting-age medical techniques including stem cell biology, regenerative medicine, and genetic technologies. Effective long-term preservation of cells holds the promise of bringing advanced cell-based techniques from laboratory to bedside of the patients. In this talk cellular engineering and biopreservation techniques will be presented from biophysical point of view. Different cellular preservation techniques will be discussed and a special emphasis will be given to an alternative approach to preservation of cells and cellular components in a desiccated state (lyopreservation). Lyopreservation offers the possibility to store cells and cellular components at non-cryogenic temperatures. Importance of biocharacterization of intracellular environment will be discussed and hyperspectral imaging technique based on confocal Raman microspectroscopy will be discussed.

Apr 25, 2016 10:40 AM Room 1011, EB1	**Dr. Grant Willson** University of Texas

Polymers for High Resolution Imaging Applications

McCabe Lecture

There has been a continuing and nearly frantic effort on the part of the microelectronics manufacturers over the past several decades to make smaller and smaller devices. Companies that cannot keep pace with these advances quickly disappear from the market place and sadly many with famous names like Siemens, Motorola and Sony have fallen by the wayside. Photolithography, the process that has enabled the production of all of today's microelectronic devices has now reached physical limits imposed by mass transport and kinetic issues. Efforts to push that technology to provide still higher resolution by the historical paths of wave length reduction, increasing the numerical aperture and reduction in the Raleigh constant have been abandoned. Is this the end? Can device scaling continue??

Various incredibly clever tricks based on chemical engineering principles have been devised by that extend the resolution limits of photolithography, some of which are already in use in full scale manufacturing. One promising approach for future generations of devices is based on the directed self-assembly of block co-polymers. We have tried to design block co-polymers that are optimized for this application. Doing so requires blocks with very high interaction parameters (c) and for some applications, incorporation of silicon into one of the blocks. Polymers of this sort form very small structures. We have now demonstrated well resolved 50 Angstrom wide lines and spaces, but aligning the structures and orienting them in a way that is useful for microelectronics is still a challenge. A progress report on these efforts will be presented.