University of Florida
College of Engineering
Department of Chemical Engineering
Graduate Association of Chemical Engineers

Tenth Annual
Graduate Association of Chemical Engineers
Graduate Symposium

February 17, 2009

Particle Engineering Research Center
Particle Science and Technology – Room 202

http://grace.che.ufl.edu
Tenth Annual Graduate Association of Chemical Engineers Graduate Symposium

February 17, 2009

Particle Science and Technology – Room 202

8:40 – 8:45 Welcome and opening remarks
Jeffery M. Hawkins, GRACE Academic Chair; and Beverly B. Hinojosa, GRACE President

Session 1: Surface Science and Advanced Materials
Judges: Dr. Jennifer Curtis and Dr. Peng Jiang

8:45 – 9:00 Jeffery M. Hawkins
Dr. Aravind Asthagiri
A density functional theory study of the initial oxidation of the Pt(111) surface

9:00 – 9:30 Heywood H. Kan
Dr. Jason Weaver
Pd(111) oxidation kinetics: Temperature and oxygen pressure effects on thin-film growth, thickness, and morphology

9:30 – 9:45 José A. Hinojosa, Jr.
Dr. Jason Weaver
STM study of high-coverage structures of atomic oxygen on Pt(111)

9:45 – 10:15 Dojun Kim
Dr. Timothy Anderson
Chemical vapor deposition of WN_xC_y using diphenylhydrazido complex Cl_4(CH_3CN)W(NNPh_2)E: Effect of NH_3 on film properties

10:15 – 10:30 Beverly B. Hinojosa
Dr. Aravind Asthagiri
Atomic displacement pathways in bismuth pyrochlores

10:30 – 11:00 Oh Hyun Kim
Dr. Timothy Anderson
Atomic layer deposition of GaN using GaCl_3 and NH_3

11:00 – 1:00 Lunch

Session 2: Complex Fluids and Biological Processes
Judges: Dr. Anuj Chauhan and Dr. Sergey Vasenkov

1:00 – 1:15 Rahul Kekre
Dr. Tony Ladd
Dr. Jason Butler
Comparing the static and dynamic properties of a semi-flexible polymer using lattice Boltzmann and Brownian dynamic simulations

1:15 – 1:30 Gaurav Misra
Dr. Richard Dickinson
Dr. Tony Ladd
Mechanics of an ultrafast cellular contraction
1:30 – 2:00  Joontaek Park  
Dynamics of rigid rodlike polymer with hydrodynamic interactions  
Dr. Jason Butler

2:00 – 2:15  Robert Russell  
Mechanics of stress fiber sarcomeres in living cells  
Dr. Tanmay Lele  
Dr. Richard Dickinson

2:15 – 2:30  Hyun-Ok Park  
Dynamics and irreversibility of oscillating suspensions of non-Brownian sphere  
Dr. Jason Butler

2:30 – 3:00  Randy K. Wang  
Enhancing the fluorescence emission of single-walled carbon nanotubes by reorganizing the surfactant structure via liquid-liquid interactions  
Dr. Kirk Ziegler

3:00 – 3:15  Break

Session 3: Biological Processes and Transport Phenomena  
Judges: Dr. Richard Dickinson and Dr. Tanmay Lele

3:15 – 3:30  Young-Min Ban  
Elastic properties of lipid bilayers containing embedded nanoparticles  
Dr. Dmitry Kopelevich

3:30 – 3:45  Cheng-Chun Peng  
Extended ophthalmic drug delivery from silicone-hydrogel contact lenses with diffusion barriers  
Dr. Anuj Chauhan

3:45 – 4:00  Nicholas Linn  
Novel “nanoflask” particles for drug delivery and therapeutics  
Dr. Peng Jiang

4:00 – 4:15  Chhavi Gupta  
Delivery of Cyclosporin A through puncta plugs and conjunctival inserts  
Dr. Anuj Chauhan

4:15 – 4:30  Brett Howell  
The mechanism of cationic drug binding to liposomes deduced from liposome leakage, drug binding, and double layer theory  
Dr. Anuj Chauhan

4:30 – 4:45  Hyun Jung Jung  
Dispersion of PGT microparticles in HEMA contact lenses for ophthalmic drug delivery  
Dr. Anuj Chauhan

4:45 – 5:00  Amrish R. Menjoge  
Nanoscale heterogeneity in systems with oppositely charged polymeric ions studied by pulsed field gradient (PFG) NMR with ultra-high gradients  
Dr. Sergey Vasenkov

5:05 – 5:15  Awards ceremony and closing remarks  
Jeffery M. Hawkins, GRACE Academic Chair; and Beverly B. Hinojosa, GRACE President
Elastic properties of lipid bilayers containing embedded nanoparticles

Young-Min Ban
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Advisor: Dr. Dmitry Kopelevich

In this talk, we discuss interactions between lipid membranes and nanoparticles. Understanding these interactions is important for development of biomimetic devices and assessment of potentially harmful effects of nanomaterials on living cells. We use molecular dynamics simulations to assess changes of elastic properties of a lipid membrane in response to embedding nanoparticles into the membrane. The considered elastic properties include the membrane bending and tilt moduli, as well as the lateral pressure profile inside the membrane. The studies are performed using a coarse-grained molecular dynamics model, which represents groups of several atoms as united atoms (beads). The considered bilayer is composed of Dipalmitoylphosphatidylcholine (DPPC) lipids. Several coarse-grained models for nanoparticles are considered in order to mimic carbon-based nanoparticles of different shapes and sizes. The considered nanoparticles are hydrophobic and therefore they reside in the interior of the bilayer. It is observed that the membrane bending modulus remains constant at moderate concentrations of nanoparticles within the bilayer. Moreover, the tilt fluctuations of the lipid molecules are affected only in the direct neighborhood of the nanoparticles. In contrast, the lateral pressure profiles change significantly upon embedding of the nanoparticles. We develop a theoretical model to explain the changes of the pressure profiles in the presence of the nanoparticles and discuss possible implication of the altered pressure profile on biophysical processes in cellular membranes.

About the speaker:

Young-Min received her Bachelor of Science from Yonsei University in Seoul, Korea, in February 2002. She continued her studies at Yonsei University by examining the effect of naphthalene on the adhesion of P. putida NCIB 9816-4 to soil surfaces and received her Master of Science in February 2004. She joined the Department of Chemical Engineering at the University of Florida in August 2005.
Currently 30 million people in US suffer from dry eyes. Therefore, devising novel methods to deliver drugs effectively is an area of prevalent research. Currently eye drops are the most common treatment of dry eyes, but problem with eye drops are their poor patient compliance and low bioavailability due to their removal from eyes through tear drainage. The tears are drained from the eyes through an opening in the eye called as puncta. Puncta plugs are designed which contain embedded drug particles that apart from blocking the puncta can also release drug such as cyclosporin A to cure the dry eyes. Also we have designed conjunctival inserts, which can be placed in conjunctival sac of the eyes, to deliver cyclosporin A. Plugs and inserts are made from HEMA (hydroxy ethyl methacrylate) coated with EGDMA (ethylene glycol dimethacrylate) to control the amount of drug release. Devices prepared are made of bio-compatible materials and can release Cyclosporin A at zero order for more than 15 days. Several in vitro experiments have been conducted to study the effect of drug concentration in the core and the effect of length of the inserts on drug release. The plugs or the inserts do not have any initial burst of drug, therefore there would be no problem of over dosage while using these devices. Also we have proposed a mechanism for the drug release from the inserts. The model simulated compares well with experimental results.

About the speaker:

Chhavi completed his undergraduate studies at the Indian Institute of Technology Guwahati in May 2006 then joined the Department of Chemical Engineering at the University of Florida in August 2006.
A density functional theory study of the initial oxidation of the Pt(111) surface

Jeffery M. Hawkins
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Advisor: Dr. Aravind Asthagiri

We used density functional theory (DFT) calculations to examine the initial stages of oxidation of the Pt(111) surface. Our calculations predict that oxygen atoms form p(2×2) and p(2×1) structures at coverages of 0.25 and 0.50 ML, respectively. In addition to various surface configurations, we also examined subsurface oxygen and clustering of oxygen atoms on the surface. We find that subsurface oxygen is not the precursor to oxidation. Instead, we predict a strong preference for the formation and growth of one-dimensional Pt oxide chains within the p(2×1) structure. In particular, oxygen atoms prefer to aggregate between the close-packed oxygen rows formed by the p(2×1) structure and induce large buckling and modification of the charge of the surface Pt atoms. The result is an oxide compound with threefold and fourfold Pt-O coordination that grows as a one-dimensional chain running parallel to the oxygen rows of the p(2×1) structure. Our results agree well with a recent STM study and suggest a novel precursor mechanism to the oxidation of metal surfaces involving Pt oxide chain formation and growth on terraces at moderate oxygen coverages.

About the speaker:

Jeff received his Bachelor of Science in chemical engineering with a polymer specialization and minors in chemistry and mathematics from the University of Akron in May 2005. He joined the Department of Chemical Engineering at the University of Florida in August 2005.
Atomic displacement pathways in bismuth pyrochlores

Beverly B. Hinojosa
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Advisor: Dr. Aravind Asthagiri

There is considerable interest in pyrochlore systems ($A_2B_2O_7$) for use in high-permittivity dielectrics, capacitors, and high-frequency filter applications. The properties of these materials can be tuned through substitutions on the A and B cation sites, resulting in an extensive parameter space. Better understanding of the role of the local atomic structure and dynamics on the macroscopic properties will enable rational design within the vast number of possibilities. Using density functional theory (DFT), quantum mechanical calculations were performed to examine several Bi-containing pyrochlores with the Fd-3m (No. 227) space group to determine the role of chemical substitutions on the local geometric and electronic structure. We considered six simple bismuth pyrochlores ($Bi_2B^{4+}_2O_7$ with $B^{4+}$ = Ti, Ru, Rh, Ir, Os, and Pt) and four pyrochlores with cation substitution selected based on availability of experimental IR and Raman spectroscopy ($Bi_{3/2}M^{2+}_{3/2}Nb_{3/2}O_7$ and $Bi_{3/2}M^{2+}_{3/2}Ta_{3/2}O_7$ with $M^{2+}$ = Zn, Mg). We will present DFT results on the structural properties of the simple pyrochlores including equilibrium lattice constants, oxygen positional parameters, and atomic displacement patterns. For the pyrochlores with cation substitution, energetics related to cation ordering will be presented, as well as atomic displacement magnitudes and pathways. Where possible, our DFT results will be compared to available experimental studies to understand the role of the atomic substitutions on the material properties.

About the speaker:

Beverly joined the Department of Chemical Engineering at the University of Florida in August 2005 after receiving her Bachelor of Science from the University of Houston’s Department of Chemical Engineering with a minor in Chemistry.
The oxidation of transition metal surfaces involves the development of a variety of oxygen states which can have distinct properties. In particular, different surface oxygen states can have unique reactive properties, which could dramatically alter the catalytic behavior of a transition metal surface. In this study we used scanning tunneling microscopy (STM) to investigate the development of oxygen structures on the Pt(111) surface under ultrahigh vacuum (UHV) conditions. We observed that oxygen atoms arrange into a p(2×1) structure that grows in three rotationally degenerate domains as oxygen coverages increase beyond 0.25 ML (monolayers). At coverages above 0.40 ML protrusions and chain-like structures begin to develop within the p(2×1) domains. These features are attributed to the initial growth of a Pt oxide chain compound that forms as oxygen atoms adsorb between the rows of the surrounding p(2×1) structure. As the coverage increase to 0.75 ML these chains form an interconnection network of Y-shaped structures, which are composed of two to three side-by-side Pt oxide chains. These results demonstrate the structural evolution of intermediate oxygen states on the Pt(111) surface and provide new insights for understanding the oxidation of Pt surfaces.

About the speaker:

José joined the Department of Chemical Engineering at the University of Florida in August 2005 after receiving his Bachelor of Science from the University of Houston’s Department of Chemical Engineering with a minor in Chemistry.
Interactions between tricyclic antidepressant drugs or the amide local anesthetic bupivacaine and anionic, pegylated liposomes designed for drug overdose treatment were studied through the use of drug binding measurements, calcein leakage from liposomes, and modeling based on electrostatic double layer theory. The experiments and modeling indicate that electrostatic interactions are responsible for the initial association between antidepressants and liposomes, whereupon the drug enters the bilayer with its charged region closely associated with the charged lipid head groups and possibly the surrounding aqueous phase as well, and its lipophilic region closely associated with the lipid bilayers. Bupivacaine, which is predominantly in the protonated state at pH 7.4 and 25°C as well (86%), is also preferentially attracted to the charged vesicle. Once bound, it appears to be located within the bilayer to a greater extent than the antidepressants, although it is likely aligned so that electrostatic interactions are maximized as well. The antidepressants have distinct hydrophilic and lipophilic regions associated with their structures, whereas the structure of bupivacaine makes it less able to access the bulk aqueous phase surrounding or encompassed by the lipid bilayers.

About the speaker:

Brett graduated from North Carolina State University in 2006 with degrees in chemical and textile engineering. He joined the Department of Chemical Engineering at the University of Florida in August 2006 and began working for Dr. Chauhan in January 2007. His work has focused on drug overdose treatment with liposomes and more generally on solving transport problems involving physiology.
Dispersion of PGT microparticles in HEMA contact lenses for ophthalmic drug delivery

Hyun Jung Jung
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Advisor: Dr. Anuj Chauhan

Ophthalmic drug delivery by eye-drops is inefficient because of low bioavailability. Only about 5% or less of the drug is absorbed into the cornea, and the remaining 95% of the drug enters the blood stream, which could lead to serious side effects. We have explored particle-laden contact lenses for ophthalmic drug delivery to increase bioavailability and to provide extended drug release. The design is based on polymerization of highly crosslinked propoxylated glyceryl triacrylate (PGT) microparticles containing timolol, a common glaucoma drug. Due to high crosslinking, the particles are expected to release drug for extended period of time. The drug-loaded particles are dispersed in polyhydroxy-ethyl methacrylate (p-HEMA) and silicone hydrogels, which are common contact lens materials. In both cases, the gels can release timolol in Dulbecco’s phosphate buffered saline (PBS) for an extended period of time lasting 3~4 weeks at therapeutic dose, which is promising for extended drug release applications. The effect of highly crosslinked particle loading on the properties of gels relevant to their use as contact lenses material such as water content and mechanical property are also studied.

About the speaker:

Hyun Jung received a Master of Science from the Department of Chemical and Biological Engineering at Korea University in 2006 then joined the Department of Chemical Engineering at the University of Florida in August 2007.
Pd(111) oxidation kinetics: Temperature and oxygen pressure effects on thin-film growth, thickness, and morphology

Heywood H. Kan
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Advisor: Dr. Jason Weaver

In this study, we characterized the oxidation of Pd(111) by utilizing a gas-phase oxygen atom beam to simulate high oxygen pressures, while still maintaining the ultrahigh vacuum conditions necessary for high precision surface characterization techniques including TPD (temperature programmed desorption), XPS (x-ray photoelectron spectroscopy), and LEED (low energy electron diffraction). We found that Pd(111) readily oxidizes at substrate temperatures as low as 100 K which suggests that the rate limiting step for oxidation is dissociative adsorption of molecular oxygen regardless of the extrinsic substrate phase. The oxidation of Pd(111) generally proceeds through oxygen chemisorption, followed by the formation of two-dimensional oxides. Then, a metastable bulk oxide precursor state forms followed finally by the formation of bulk oxide. We observed a strong dependence of oxide film thickness on incident flux and substrate temperature, with final film thicknesses increasing with increasing substrate temperature or decreasing incident flux. We also observed drastic differences between high temperature and low temperature oxidation kinetics, with the transition between high and low temperature oxidation being abrupt over a very narrow temperature window within the bulk oxide precursor state thermal instability range. Finally, we will present arguments that the precursor to bulk oxide formation represents chemically distinct oxide “seeds” which coexist with the two-dimensional surface oxide, with their thermal stability well described with the Kelvin Equation. This model for oxide growth is supported by numerical simulations which adequately reproduce the uptake behavior observed experimentally. Overall, the work presented herein provides a context for understanding the kinetics of catalytic oxidation reactions over palladium and other late-transition metal catalysts.

About the speaker:

Heywood received his Bachelor of Science in chemical engineering from the University of California at Berkeley, where he did undergraduate research under both Dr. D.V. Schaffer and Dr. D.B. Graves. He also worked at the Public Utilities Commission of San Francisco as a process engineer during an undergraduate co-op. He joined the Department of Chemical Engineering at the University of Florida in August 2004. During his time here, he has published 11 manuscripts in peer-reviewed journals in addition to giving 4 presentations at international conferences. After graduation, he will be traveling to Hillsboro, Oregon, to begin work at Intel.
Comparing the static and dynamic properties of a semi-flexible polymer using lattice Boltzmann and Brownian dynamic simulations

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Advisor: Dr. Tony Ladd and Dr. Jason Butler

We simulate a linear semi-flexible polymer using lattice Boltzmann and Brownian dynamics techniques. Polymer conformations are studied for multiple parameters like the time step size, the box length and the resolution of the lattice grid. The static properties, namely the radius of gyration ($R_g$) and end to end vector ($R_e$), are reported and are within 1% of one another. Extensive comparisons of the dynamics of the polymer chain are made by measuring its diffusivity and Rouse relaxation times. The monomer radius, $a$, and grid spacing, $\Delta x$, affect the hydrodynamic correlations at large temporal scales in the lattice-Boltzmann simulations. By choosing a monomer radius of $a < 0.2\Delta x$ and using the value of the grid resolution as $\Delta x/b = 1.00$ as suggested by [P. Ahlrichs and B. Dünweg, J. Chem. Phys. 111, 8225 (1999)], we can map the lattice-Boltzmann results for the Rouse relaxation times and the diffusivity of the polymer to the corresponding values obtained by the Brownian dynamics calculations. The lattice-Boltzmann results are insensitive to the temperature of the system and thus suggest the absence of any retardation effects due to inertia. Our work complements an independent study [T. T. Pham, U. D. Schiller, J. R. Prakash, and B. Dünweg, to be published] that also found favorable matching of the static and dynamic properties of a flexible polymer using lattice Boltzmann and Brownian dynamics.

About the speaker:

Rahul completed his undergraduate studies at the Indian Institute of Technology Bombay in 2005 then joined the Department of Chemical Engineering at the University of Florida in August 2006.
Chemical vapor deposition of WN\textsubscript{x}C\textsubscript{y} using diphenylhydrazido complex Cl\textsubscript{4}(CH\textsubscript{3}CN)W(NNPh\textsubscript{2}): Effect of NH\textsubscript{3} on film properties

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Advisor: Dr. Timothy Anderson

The tungsten diphenylhydrazido complex Cl\textsubscript{4}(CH\textsubscript{3}CN)W(NNPh\textsubscript{2}) \cite{1} was used for film growth of tungsten carbonitride (WN\textsubscript{x}C\textsubscript{y}) thin films by metal-organic chemical vapor deposition (MOCVD) in the absence and presence of ammonia (NH\textsubscript{3}) in H\textsubscript{2} carrier. The effect of deposition temperature and NH\textsubscript{3} on the film microstructure, chemical composition, bonding states, surface morphology, growth rate, and electrical resistivity were studied. The microstructure of films deposited with NH\textsubscript{3} was X-ray amorphous below 450°C. The chemical composition of films deposited with NH\textsubscript{3} exhibited the increased N levels between 400 and 700°C and decreased C levels at and below 400°C as compared to films deposited without NH\textsubscript{3}. As determined by XPS, W is primarily bonded to N and C for films deposited between 300 and 700°C, but even if at lower deposition temperature (< 400°C) the binding energy of the W-O bond becomes less evident. Growth rates varied from 7.3 to 14.3 Å/min without any transition point in the growth regime. Diffusion barrier properties were investigated to determine the performance of the diffusion barrier. Cu/WN\textsubscript{x}C\textsubscript{y}/Si stacks annealed at 500°C for 30 min maintained the integrity of both Cu/WN\textsubscript{x}C\textsubscript{y} and WN\textsubscript{x}C\textsubscript{y}/Si interfaces. Cross-sectional TEM images show that there is no Cu diffusion through WN\textsubscript{x}C\textsubscript{y} and Si. EDS qualitative analysis shows that Cu K\alpha peak decreases sharply at the Cu/WN\textsubscript{x}C\textsubscript{y} interface. Hence, WN\textsubscript{x}C\textsubscript{y} thin films deposited at 400°C are a viable material to serve as a Cu diffusion barrier. The film properties of thin films deposited with \cite{1} and tungsten imido complexes Cl\textsubscript{4}(CH\textsubscript{3}CN)W(NR) (R = Ph, iPr, and allyl) were also compared to provide insight into the effect of hydrazido and imido ligands on film properties.

About the speaker:

Dojun completed his undergraduate studies in chemical engineering at Seoul National University in 1998. He received his master’s degree from Seoul National University in 2000, and then worked as a process engineer at SK Engineering & Construction until 2005. He joined the Department of Chemical Engineering at the University of Florida in August 2005.
Atomic layer deposition of GaN using GaCl$_3$ and NH$_3$

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Advisor: Dr. Timothy Anderson

GaN films were grown on Si(100) substrate by atomic layer deposition (ALD) using GaCl$_3$ and NH$_3$. Growth conditions were identified for which the growth rate exhibited a plateau at ~2.0 Å/cycle consistent with self-limiting adsorption. A relatively wide temperature window (500 to 750°C) for ALD growth mode was also established for one flow sequence schedule. In this limit, both the (002) and (101) orientations of GaN were evident, which was attributed to the competition between vertical and lateral growth. Chlorine incorporation was detected by XPS for samples prepared with long GaCl$_3$ exposure time. It is postulated that gas phase formation of (ClGaNH)$_n$ with n = 1-3 results in higher chlorine content.

About the speaker:

Oh Hyun received his Bachelor of Science in chemical engineering from Seoul National University in 2004. He then joined the Department of Chemical Engineering at the University of Florida in August 2004.
Novel “nanoflask” particles for drug delivery and therapeutics

Nicholas Linn
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Advisor: Dr. Peng Jiang

Synthesis and characterization of novel multifunctional nanostructures for photothermal drug delivery and therapeutics is reported. Using spin coating of silica nanoparticles, metal sputtering, and reactive ion etching, an ordered array of hollow gold flask-shaped nanoparticles with tunable size and pore diameter is generated. A layer of a magnetic material can be added and the dimensions of a nanoflask particle can be modified such that the particle exhibits a surface plasmon resonance at near-IR frequencies. Fluorescence microscopy shows that the nanoflasks can be filled with a heat sensitive active drug carrying matrix, thereby allowing controlled drug release on exposure to near-IR light. Preliminary results for photothermal drug release will be shown. Fabrication yields a bare gold surface which can be easily functionalized with antibodies or PEG and thus particles can be used for MRI contrast, as drug delivery vehicles, and as photothermal ablation agents.

About the speaker:

Nicholas received his Bachelor of Science in chemical engineering and Bachelor of Arts in chemistry from North Carolina State University in 2006. He joined the Department of Chemical Engineering at the University of Florida in August 2006.
Nanoscale heterogeneity in systems with oppositely charged polymeric ions studied by pulsed field gradient (PFG) NMR with ultra-high gradients

Amrish R. Menjoge
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Advisor: Dr. Sergey Vasenkov

Nanoscale heterogeneity arising due to interaction between oppositely charged polymeric ions is common in many systems of industrial importance such as room temperature ionic liquids and polyelectrolyte coacervates. The nature and properties of the microscopic heterogeneities can determine many macroscopic properties of these systems. Hence, understanding the nanostructural organization in such substances holds the key to their applications.

Polypelectrolyte coacervates are formed by oppositely charged polycation and protein molecules (active ingredient). They have a potential for applications in protein encapsulation. It has been hypothesized that the coacervate structure exhibits microscopic dense domains rich in protein and polycations dispersed in a lower density fluid phase. Ionic liquids (ILs) are organic salts that are molten at temperatures below 100°C and have many unique properties, which include negligibly small vapor pressure, ability to act as good industrial solvents, good thermal stability and electrical conductivity. Such commercially potent properties of ILs are thought to arise from formation of microscopic polar and nonpolar domains formed by the oppositely charged ions.

In the presented work, PFG NMR diffusion studies with ultra-high magnetic field gradients (up to 30 Tm⁻¹) were carried out to study dynamics and nanostructural organization in the systems mentioned above. PFG NMR is a noninvasive technique which permits in situ dynamic studies of various species on length scales of molecular displacements as small as 90 nm as well as on much larger length scales. Our research group is the only one in United States that has developed a proven capability to use such high gradient strengths for diffusion studies under the conditions of application of very high (17.6 T) magnetic field.

About the speaker:

Amrish received his Bachelor of Science in chemical engineering from the Mumbai University Institute of Chemical Technology in 2004. He then joined the Department of Chemical Engineering at the University of Florida in August 2004, where he received his Master of Science in chemical engineering in 2005.
Mechanics of an ultrafast cellular contraction

Gaurav Misra
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Advisors: Dr. Richard Dickinson and Dr. Tony Ladd

Vorticella Convallaria is one of a class of fast-moving organisms, traversing its body size in less than a millisecond. It has two main parts, the cell body and a stalk, which attaches the cell body to the substrate. The stalk houses a slender, elastic structure called Spasmoneme, which winds helically inside the stalk and generates a strong tensile force in response to Calcium signaling. We are developing numerical simulations of the collapsing stalk to quantify the role of different processes operating at different time scales. We have coupled a Kirchhoff model of an elastic rod (representing the stalk) with an embedded helically wound filament (representing the Spasmoneme).

Contraction of this assembly is driven by a constant velocity Calcium signal that induces a state of tension in the Spasmoneme. Depending on the speed of the Calcium signal, we observe different mechanical responses from the contracting stalk, which we compare with experimental observations. We follow the interplay of contraction, twist and bend to explain some features of the contraction process. We have also identified the geometric constraints that the system of stalk and Spasmoneme must satisfy in the process of contraction. These geometric constraints enable us to predict the configuration of the contracted Vorticella for given parameters.

About the speaker:

Gaurav received his B.Tech. in chemical engineering from the Indian Institute of Technology Bombay in 2003, then worked as in IT consultant for Deloitte Consulting in India until February 2005. He then joined the Department of Chemical Engineering at the University of Florida in August 2005, where he is working on multi-scale modeling and simulation of filaments, particularly actin. Gaurav enjoys clear blue skies and homemade cookies.
Dynamics and irreversibility of oscillating suspensions of non-Brownian sphere

Hyun-Ok Park
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Advisor: Dr. Jason Butler

The dynamics and irreversibility of a suspension of non-Brownian spheres is studied using oscillatory rheology. The complex viscosity of the suspensions demonstrates a non-monotonic dependence on strain amplitude for volume fractions larger than 0.2. The measurements of changes in the complex viscosity are indicative of changes in the underlying microstructure. Short-time and long-time rheology was evaluated with regard to irreversibility. Although the oscillatory rheology reaches a quasi-steady state at a small number of oscillations, it shows continuing changes of the complex viscosities with total strain over long time scale. Therefore, irreversible changes of microstructures subject to the oscillatory shear flow are indicated, supported by experiments and Stokesian dynamics simulations.

About the speaker:

Hyun-Ok received a Bachelor of Science in chemical engineering from Korea University in 2001 and a Master of Science in chemical engineering from Seoul National University in 2003. After working as a researcher at DCC R&D Center in 2003 and 2004, she joined the Department of Chemical Engineering at the University of Florida in August 2005.
Dynamics of rigid rodlike polymer with hydrodynamic interactions

Joontaek Park
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Advisor: Dr. Jason Butler

Kinetic theory is developed to investigate cross-stream migration of a rigid rod-like polymer undergoing rectilinear flow in the vicinity of a wall. Hydrodynamic interactions between the polymers and the boundary result in a cross-stream migration. In simple shear flow, polymers migrate away from the wall, creating a depletion layer in the vicinity of the wall which thickens as the flow strength increases relative to the Brownian force. In pressure-driven flow, an off-center maximum in the center-of-mass distribution occurs due to a competition between hydrodynamic interactions with the wall and the anisotropic diffusivity induced by the inhomogeneous flow field.

Brownian dynamics and slender-body theory are used to simulate suspensions of rigid fibers under simple shear, pressure-driven and oscillatory shear flows between two parallel walls at zero Reynolds number and high Peclet number. The theoretical distributions are compared with the results of the simulations. The center-of-mass distributions obtained by simulations and the theory are in good agreement and confirm a net migration away from the wall. The good agreement validates approximations made in the theory, such as negligible effect of the wall on the orientation distribution.

About the speaker:

Joontaek received his Bachelor of Science in chemical engineering from Seoul National University in 1996 then his Master of Science from the Korea Advanced Institute of Science and Technology in 1998. After working as a research engineer at SK Engineering & Construction until 2004, he joined the Department of Chemical Engineering at the University of Florida in August 2004.
Ophthalmic drug delivery via soft contact lenses have been widely studied due to its high degree of comfort, biocompatibility, and significant increase in drug residence time and bioavailability compared to delivery via eye drops. However, a majority of the drugs taken up by the commercial contact lenses was released in a very short period of time, which is not suitable for extended drug release need. This study focuses on the concept of increasing the release duration of drugs from commercial silicone-hydrogel contact lenses by creation of transport barriers. Vitamin E, which is considered as an important ocular nutraceutical, is loaded in different commercially available silicone contact lenses by soaking the gels in ethanol-vitamin E solution then forming aggregates after ethanol evaporation. With negligible changes of the geometry of the lens, the vitamin E loading inside the gel effectively increases the drug delivery duration from several hours to a few weeks, especially for hydrophilic drugs such as timolol, fluconazole and dexamethasone 21-disodium phosphate (DXP). The effect is smaller for release of hydrophobic drugs such as dexamethasone (DX) and ketotifen fumarate (KF). Since hydrophilic drugs are almost insoluble in vitamin E, the drugs inside the gels have to diffuse around the vitamin E aggregates, leading to an increase in effective path length, and thus an increase in the duration of the drug release. A scale theory is established to explain the quadratic relationship between the hydrophilic drug release time increase and the volume fraction of vitamin E in the lenses.

About the speaker:

Cheng-Chun received a Bachelor of Science in chemical engineering from National Taiwan University in 2003, continued studies for a Master of Science in 2005, and then joined the Department of Chemical Engineering at the University of Florida in August 2007.
Mechanics of stress fiber sarcomeres in living cells

Robert Russell
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Advisor: Dr. Tanmay Lele and Dr. Richard Dickinson

Actin filaments inside endothelial cells assemble into tensed bundles called stress fibers. Stress fibers are observed in vivo in a variety of tissues including the aorta, the heart, the spleen, the eye, and hair follicles. Sarcomeres are the force generating units of stress fibers and are responsible for generating intracellular tension. Little is known about the mechanical behavior of individual sarcomeres in living cells. Using femtosecond laser ablation to sever individual stress fibers in living capillary endothelial cells, we are able to measure the mechanics of sarcomeres in living cells. Our results indicate that the length of a sarcomere after severing decreases in two phases - an initial elastic response, followed by slower contraction at constant speed. The latter phase, interpreted as active myosin-mediated contraction, ceases abruptly after a minimum sarcomere length is achieved, suggesting a rigid resistance that prevents further contraction. We model this with an equivalent mechanical circuit, allowing us to estimate the speed of myosin motor walking in sarcomeres for the first time. We find that this speed ranges from 0.02 to 0.1 μm/s, which compares well with in vitro measurements. Our analysis suggests a novel mechanical model of a sarcomere that includes an active force generating component in parallel with an infinite barrier and in series with a stiff elastic spring.

About the speaker:

Robert received his Bachelor of Science in chemical engineering and biomedical engineering from Carnegie Mellon University in spring 2006. He then joined the Department of Chemical Engineering at the University of Florida in August 2006.
Enhancing the fluorescence emission of single-walled carbon nanotubes by reorganizing the surfactant structure via liquid-liquid interactions

Randy K. Wang
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Advisor: Dr. Kirk Ziegler

Single-walled carbon nanotubes (SWNTs) have a unique near-infrared fluorescence associated with their \((n, m)\) type. Single molecule microscopy experiments have shown that the quantum yields of SWNTs may be 10% or higher. However, bulk-scale suspensions typically yield quantum yields less than 1%. This discrepancy is often attributed to extrinsic factors, which quench fluorescence. These differences point to the importance in understanding how SWNT dispersion processes affect fluorescence and learning how to compensate for the extrinsic effects. Here we show that mixing aqueous suspensions with immiscible solvents is capable of reorganizing the surfactant structure surrounding SWNTs, resulting in significant increases to the fluorescence intensity (quantum yield). Solvatochromic shifts associated with the modification of the environment surrounding SWNTs suggest the hydrophobic region of the micelle swells with the organic solvent when mixed. The solvatochromic shifts of the aqueous SWNT suspensions are reversible once the solvent evaporates. However, some surfactant-solvent systems show permanent changes to the NIR fluorescence emission intensity after exposure to the organic solvent. The intensity of some large diameter SWNT \((n, m)\) types increase by more than 175%. These differences are attributed to surfactant reorganization, which can improve nanotube coverage, resulting in decreased exposure to quenching mechanisms from the aqueous phase.

About the speaker:

Randy received his Bachelor of Science in chemical engineering from National Taiwan University in June 2003 then worked as a research engineer with LCD panels at Chunghwa Picture Tubes, Ltd. in Taiwan. He then joined the Department of Chemical Engineering at the University of Florida in August 2005.
This symposium has been sponsored by
the Department of Chemical Engineering at the University of Florida

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