SOCIETY OF POSTDOCTORAL SCHOLARS
UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

SOPS.BECKMAN.ILLINOIS.EDU

4TH ANNUAL POSTDOCTORAL RESEARCH SYMPOSIUM

JANUARY 31, 2014

Beckman Foyer near Auditorium and Room 1005: Registration

8:00 – 8:45 Registration and light breakfast
Posters up

Auditorium: Opening Remarks and Keynote

8:45 – 8:50 Welcome - Society of Postdoctoral Scholars, Camille Goudeseune
8:50 – 8:55 Remarks - Postdoctoral Affairs Office
9:00 – 10:00 Keynote: Gene Robinson
The Relationship Between Genes and Social Behavior: Lessons from the Honey Bee

Beckman Foyer near Auditorium and Room 1005: Break

10:00 – 10:15 Break: Coffee, tea, water

Auditorium: Talks, Session 1 Chair: Juan Perilla

10:15 – 10:30 Juan Perilla
Molecular mechanisms of HIV infection (1.1)
10:30 – 10:45 Sarah Erickson-Bhatt
In vivo intra-operative breast tumor margin detection using a portable OCT system with a handheld surgical imaging probe (1.2)
10:45 – 11:00 Sheng Xu
Hard-soft integrated multifunctional devices for mobile healthcare systems (1.3)
11:00 – 11:15 Venkatraman Srinivasan
Fewer not more leaves - Key to obtaining the needed jump in crop yield potential (1.4)
11:15 – 11:30 Craig Yendrek
Exploiting inter-specific variation to improve abiotic stress tolerance in crops (1.5)

Beckman Foyer near Auditorium and Room 1005: Break

11:30 – 11:45 Break: Coffee, tea, water

Auditorium: Talks, Session 2 Chair: Mostafa Elag

11:45 – 12:00 Mostafa Elag
Data network (2.1)
12:00 – 12:15 Catello Di Martino
Lessons learned from the failure analysis of Blue Waters (2.2)
12:15 – 12:30 Robin Berthier
Challenges and solutions for a resilient power grid (2.3)
12:30 – 12:45 Yukako Komaki
Analyses of cell cycle alteration induced by haloacetonitriles: Toxicity of drinking water disinfection by-products (2.4)

12:45 – 1:00 Aaron Finck
Vortices and gate-tunable bound states in a topological insulator coupled to superconducting leads (2.5)

Beckman Atrium and Room 1005: Poster Session and Lunch

1:00 – 3:00 Lunch
1:30 – 2:15 Even number posters presented
2:15 – 3:00 Odd number posters presented

Auditorium: Talks, Session 3 Chair: Christopher Mayne

3:00 – 3:15 Christopher Mayne
Force field toolkit: Rapid parameterization of small molecules for use in biomolecular simulations (3.1)
3:15 – 3:30 Oya Okman
Self-healing in Li-ion battery electrodes (3.2)
3:30 – 3:45 Chi Hwan Lee
Transfer printing method for flexible, cheap and light-weight thin-film electronics (3.3)
3:45 – 4:00 Rui Zhang
Accelerated self-replication under non-equilibrium, periodic energy delivery (3.4)

Beckman Foyer near Auditorium and Room 1005: Break

4:00 – 4:15 Break: Coffee, tea, water

Auditorium: Talks, Session 4 Chair: Emmanuel Nuesiri

4:15 – 4:30 Emmanuel Nuesiri
All adaptation is local: Local government capacity and climate change (4.1)
4:30 – 4:45 Rodica Damian
Psychopathology, adversity, and creativity: Diversifying experiences in the development of eminent African-Americans (4.2)
4:45 – 5:00 Alex Konkel
They can take a hint: Preserved integration of outside information with memory in older adults (4.3)
5:00 – 5:15 Audrey Michal
The role of attentional shifts in graph comprehension (4.4)

Auditorium: Closing Remarks

5:15 Closing remarks, Ryan Gilbert-Wilson

Beckman Atrium: Reception

5:20-6:30 Reception
Audience Choice Talk, Audience Choice Poster, and Travel Awards
6:30 Remove posters

Organizers: Ryan Gilbert-Wilson, Yekaterina Golubeva, Camille Goudeseune
Taras Pogorelov, Evelina Tapia

Sponsors: Office of the Chancellor, Beckman Institute, The Institute for Genomic Biology, College of Engineering, College of Liberal Arts and Sciences, and the Graduate College

Talk abstracts

1. 1 Molecular mechanisms of HIV infection

Juan Perilla（juan@ks.uiuc.edu,） Christopher Aiken, Peijun Zhang, Klaus Schulten
Department of Physics and Beckman Institute

Antiretroviral therapies against human immunodefficiency virus type 1 (HIV-1) have reduced the mortality of infected individuals. However, the ability of the virus to acquire resistance to currently administered treatments has prompted the need for new therapies. The genome of HIV-1 is encased by a protein shell known as the capsid, which is an assymetrical cone-shaped core composed of the capsid protein CA. Although early work suggested a trivial role for the capsid during the infection process, recent data has shown that the stability and geometry of the capsid are required for several key steps during the infective cycle. In this talk we present the structure of the HIV-1 capsid, its interactions with potent anti-retroviral drugs, as well as human host factors. These findings reveal new drug targets, new drug mechanisms, and molecular details of HIV's infective cycle.

1.2 In vivo intra-operative breast tumor margin detection using a portable OCT system with a handheld surgical imaging probe

Sarah Erickson-Bhatt (serickso@illinois.edu), Ryan Nolan, Nathan D. Shemonski, Steven G. Adie, Jeffrey Putney, Donald Darga, Daniel T. McCormick, Andrew Cittadine, Marina Marjanovic, Eric J. Chaney, Guillermo L. Monroy, Fredrick South, P. Scott Carney, Kimberly A. Cradock, Z. George Liu, Partha S. Ray, Stephen A. Boppart
Beckman Institute, University of Illinois at Urbana-Champaign

Breast-conserving surgery is a frequent option for women with stage I and II breast cancer, and with radiation treatment, can be as effective as a mastectomy. However, adequate margin detection remains a challenge, and too often additional surgeries are required. Optical coherence tomography (OCT) provides a potential method for real-time, high-resolution imaging of breast tissue during surgery. In this study, a novel handheld surgical probe-based OCT system is introduced and used by the surgeon to image the tumor cavity in vivo, and immediately following tumor removal in order to detect the presence of any remaining cancer. Following resection, the excised tissue was imaged with the same probe for comparison. We present OCT images obtained from patients during lumpectomy and mastectomy surgeries. Images were compared to post-operative histopathology for diagnosis. OCT images with micron scale resolution show areas of heterogeneity and disorganized features indicative of malignancy, compared to more uniform regions of normal tissue. Video-rate acquisition shows the inside of the tumor cavity as the surgeon sweeps the probe along the walls of the surgical cavity. This demonstrates the potential of OCT for real-time assessment of surgical tumor margins and for reducing the unacceptably high re-operation rate for breast cancer patients.

1.3 Hard-soft integrated multifunctional devices for mobile healthcare systems

Sheng Xu（shengxu@illinois.edu, Yihui Zhang, Kyle Mathewson, Yonggang Huang, John Rogers
University of Illinois at Urbana-Champaign

An important trend in flexible personal electronics involves the development of materials, mechanical designs and manufacturing strategies that enable the use of unconventional substrates, such as polymer films, metal foils, paper sheets or rubber slabs. A particular challenge lies in the need for the entire system to accommodate not only bending but also stretching due to the time dynamic and curvilinear of human body. Here we introduce a set of materials and design concepts for a wearable and mechanically invisible device patch that exploits the rigid commercial off-the-shelf (COTS) surface mounted chips. This design utilizes thin soft silicone elastomer with a hierarchical relief structure as the substrate, multilayered 'self-similar' structures as interconnects, and a novel packaging scheme to isolate the strain at the hard/soft interface. The result enables a skin mounted multifunctional electronic system with reversible stretchability up to 100% and capable of wireless charging, multi-channel biological signal sensing, e.g. electrophysiological potential, temperature and motion, and RF communication to the backend receiver.

1.4 Fewer not more leaves - Key to obtaining the needed jump in crop yield potential

Venkatraman Srinivasan (vsriniv3@illinois.edu), Stephen Long, Praveen Kumar
Institute for Genomic Biology, University of Illinois

Word food and feed supply needs to increase by 75% by 2050. Soybean is the world`s fourth most important crop in terms of total production at 249 million Mt/yr and a key protein source. In common with rice and wheat, year on year global yield increases are declining and at present rates of improvement, 2050 targets cannot be reached without new innovations. Here we demonstrate an innovative approach that could provide a yield jump. Natural selection favors individual plants to maximize leaf production within the limits of their resources to maximize light interception and shade competitors. This trait from millennia of evolution carried over into our domestic crops could be disadvantageous. In addition, as we show here, rising CO2 is causing increased leaf production. Here, we show by mathematical model and field experiment that a modern cultivar growing at the center of US soy cultivation produces too many leaves and reduction to an optimal level would increase yield by between 8 and 23%. This is validated under current and future atmospheric CO2 conditions.

1.5 Exploiting inter-specific variation to improve abiotic stress tolerance in crops

Craig Yendrek (cyendrek@illinois.edu), Elizabeth Ainsworth
Plant Biology, University of Illinois

The past decade has seen tremendous advances in genomics tools, especially those related to high-throughput

DNA sequencing. This has aided geneticists in developing populations that encompass much of the existing genetic diversity for each of the major U.S. crops. Applications for these powerful genetic resources include QTL studies to identify loci related to stress tolerance as well as the integration of traits that confer stress tolerance into elite germplasm, both of which also rely on collecting high-throughput phenotypic data for agronomic traits. However, these populations cannot be screened for physiological changes in response to environmental stress because obtaining measurements of photosynthesis are prohibitively time-consuming using existing technologies. Here, I will demonstrate the feasibility of quickly estimating photosynthetic parameters from leaf optical properties in the visible, near infrared and shortwave infrared spectral regions. I will also present additional leaf characteristics, including leaf chlorophyll and water content, that were monitored using leaf reflectance spectra by screening field-grown maize exposed to elevated air pollution.

2.1 Data Network

Mostafa Elag (elag@illinois.edu), Praveen Kumar
Electrical and Computer Engineering, UIUC

Data curation is the underpinning of scientific advancements. The exponential growth in data production is spanned across Earth Science small research groups, which is termed as log-tail data, increases the data-knowledge latency among related domains. It has become clear that an advanced framework-agnostic metadata and ontologies for long-tail data is required to increase their visibility to each other, provide concise and meaningful descriptions that reveal their connectivity. The rich content, linked data, of these data networks provides unprecedented opportunities for data analysis in different scientific context that perhaps may lead to new scientific patterns. Despite the advancement that has been achieved by various sophisticated data management models in different Earth Science research domains, it is not always straightforward to reuse or derive emergent relationships among long-tail data. Semantic data clustering algorithm and pre-defined rules that are oriented toward prediction of possible data relationships, is one method to address these challenges. This work advances the connectivity of related long-tail data by introducing the design for an ontology-based knowledge management system. In this research, we present the system architecture, its components, and illustrate how it can be used to scrutinize the connectivity among datasets.

2.2 Lessons learned from the failure analysis of Blue Waters

Catello Di Martino (dimart@illinois.edu), Ravishankar Iyer, Zbigniew Kalbarczyk
Coordinated Science Laboratory, University of Illinois

This talk will present the first failure characterization study of a petascale supercomputers. System administrators report on failures and event logs collected over 261 days are used to characterize failures. The characterization is performed by i) looking for how failures break down in root causes, ii) considering what failures cause system-wide outages, and iii) providing a direct assessment of memory, processor, network, GPU accelerator and file system resiliency to error. The major findings of this study are: (i) while hardware is the primary contributor to the total number of failures (42\%), failures due to hardware causes are responsible for only 23\% of the total repair time, (ii) software is the major contributor to the total repair time (53\%), despite being the cause of only 20\% of the total number of failures; (iii) the Lustre file system is the most critical component in Blue Waters causing as much as 62\% of system-wide outages, with 42\% of them being caused by failures of the automated failover procedures; and (iv) the memory protection mechanisms utilized in the machine (Chipkill, ECC, and parity) are effective in correcting 99.997\% of the errors, failing in only 28 of the 1,564,024 analyzed errors.

2.3 Challenges and Solutions for a Resilient Power Grid

Robin Berthier (rgb@illinois.edu), Katherine R. Davis, Charles M. Davis, Rakesh B. Bobba, Saman Zonouz, Peter W. Sauer
Information Trust Institute, University of Illinois

The electric grid has been ranked the greatest technological achievement of the 20th century by the National Academy of Engineering. In the contiguous US only, the electric power transmission consists of 300,000 km of lines operated by 500 companies. With the advances in communication capabilities brought by the 21st century, the power grid is being actively upgraded into a “smart grid” where two-way communications and intelligent devices help to improve the reliability of the system and to save energy. This presentation will explain some of the challenges and solutions to make sure that the upgraded grid remains highly resilient against accidental and intentional failures.

2.4 Analyses of Cell Cycle Alteration Induced by Haloacetonitriles: Toxicity of Drinking Water Disinfection by-Products

Yukako Komaki (ykumada@illinois.edu), Benito J. Marinas, Michael J. Plewa
Civil and Environmental Engineering, UIUC

The introduction of drinking water disinfection greatly suppressed outbreaks of waterborne diseases. Yet, epidemiological studies have associated the disinfected water consumption with slightly elevated risk for bladder cancer and adverse pregnancy outcomes. While over 600 disinfection by-products (DBPs) have been identified, the precise mechanisms of tumor induction by the complex mixtures of DBPs in disinfected water are still unknown. Haloacetonitriles (HANs) are a chemical class of DBPs and demonstrated be mutagenic, genotoxic, clastogenic and developmentally toxic. Treating Chinese hamster ovary (CHO) cells with monoHANs followed by the release from the treatment resulted in accumulation of high ploidy cells over time. It appeared that HANs adversely affected the cell cycle progression by interfering with mitosis. Presumably HAN-treated cells underwent another cell cycle and became tetraploid, and further progression of cell cycle resulted in induction of high ploidy cells. There are accumulating evidences of transient tetraploid state proceeding aneuploidy in cancer progression. It is possible that HAN disruption of the normal cell cycle and the generation of aberrant cells with abnormal number of chromosomes may contribute to cancer induction and adverse health outcomes associated with consumption of disinfected water.

2.5 Vortices and gate-tunable bound states in a topological insulator coupled to superconducting leads

Aaron Finck (afinck@illinois.edu), Cihan Kurter, Y.S. Hor, Dale Van Harlingen
Department of Physics, UIUC

Topological superconductors are unusual materials that host exotic states bound to topological defects, such as vortices. These exotic states, often referred to as Majorana fermions, can encode and process quantum information non-locally; thus, they can implement a special type of quantum computer that is robust against decoherence. Here, we seek to engineer a topological superconductor by coupling a topological insulator (bismuth selenide) to a conventional superconductor (niobium). Superconductivity can leak into the bismuth selenide from the niobium, leading to a correlated state that can act like a topological superconductor. We perform transport studies of the resulting heterostructure by driving electrical current into it from a normal metal lead. When a large magnetic field is applied, we find abrupt changes in the transport at very specific magnetic fields. Remarkably, these shifts are accompanied by very sharp spikes in the resistance at bias currents that are extremely sensitive to tiny changes in the magnetic field. We interpret these transitions as being signatures of vortices nucleating within the engineered topological superconductor due to the magnetic field. Finally, at high magnetic fields, we also find evidence of bound states whose energies can be tuned by an electrostatic back gate.

3.1 The Force Field Toolkit: Rapid Parameterization of Small Molecules for Use in Biomolecular Simulations

Christopher Mayne (cmayne2@illinois.edu), Saam, K. Schulten, J.C. Gumbart, and E. Tajkhorshid
Beckman Institute, UIUC

The maturation of molecular dynamics (MD) through much technological advancement to extend the system size and simulation timescale remains the driving force in enabling methods to probe biological systems. An often-overlooked, but serious and long-persisting limitation, however, is the complexity of developing missing force field parameters for novel chemical matter, such as modified amino acids or small molecule ligands. To directly address this unmet need, we have developed the Force Field Toolkit (ffTK) for the development of force field parameters from first principles with a specific focus on small molecules. Written entirely in Tcl/Tk and distributed as a VMD plugin, users interact with the toolkit via a graphical user interface that formalizes each step of the parameterization, and organizes them into a clear, modular workflow. Computations leverage a selection of optimization algorithms with access to an array of settings. A unique aspect of ffTK is the inclusion of embedded analysis utilities to quantitatively assess the progress of the optimization, and the performance of the resulting parameters. We have applied these tools to benchmark several classes of molecules against parameters available in the existing MD force fields, and will discuss the results herein.

3.2 Self-healing in Li-ion battery electrodes

Oya Okman (okman@illinois.edu), Sen Kang, Scott R. White, Nancy R. Sottos
Beckman Institute, Department of Materials Science and Engineering, Department of Aerospace Engineering, UIUC

Battery lifetime relies on the electrical and mechanical integrity of its electrodes. During subsequent charging and discharging cycles in a standard battery operation, the electrodes experience high mechanical stress leading to cracks and eventually capacity loss. This is a common cause of degrading battery performance. In this study, we capture cracking of graphite based electrodes during cell operation and introduce a microcapsule based self-healing approach to restore functionality of the electrode. We incorporate microcapsules with a conductive core in the electrode, which deliver their content locally at the damage zone and restore conductance across newly-formed cracks. We first enhance localized electrode cracking by including stress concentration zones in the electrode design, and thus, induce a capacity loss based on mechanical failure and then observe autonomous restoration of battery capacity during its regular operation.

3.3 Transfer Printing Method for Flexible, Cheap and Light-weight Thin-Film Electronics

Chi Hwan Lee (chihwan@illinois.edu), Xiaolin Zheng
Materials Science and Engineering, University of Illinois at Urbana-Champaign

Thin-film electronics on non-silicon based cheap/flexible substrates, such as papers, plastics, clothes, etc., possess the advantage of mechanical flexibility in actual use and lower manufacturing cost associated with roll-to-roll fabrication. However, use of the flexible, cheap and light-weight substrates has been limited by process temperature as well as incompatibility with conventional CMOS fabrication facilities. Here, we present a new and simple transfer printing method for the transfer of diverse thin-film electronics to flexible, cheap and light-weight substrates without degradation in device performances. To demonstrate, we have successfully transferred thin-film transistors (TFTs) and thin-film solar cells (TFSCs) which are pre-fabricated on a silicon wafer onto various nonconventional yet useful substrates, such as plastics, papers, adhesive tapes, aluminum foil, etc. Key features of this approach are that the transfer process only takes about a few seconds in water at room temperature, and the transfer yield is nearly 100%. Based on the simplicity, low-cost, and scalability of our transfer printing method, we believe that it can be applied to industry with little barrier, but also easily applied to other thin-film Si based transistors.

3.4 Accelerated Self-Replication under Non-Equilibrium, Periodic Energy Delivery

Rui Zhang (rzhang9@illinois.edu), David Walker, Bartosz Grzybowski, Monica Olvera de la Cruz
Materials Science and Engineering, UIUC

Self-replication is a remarkable phenomenon in nature that has fascinated scientists for decades. In a self-replicating system, the original units are attracted to a template, which induce their binding. In equilibrium, the energy required to disassemble the newly assembled copy from the mother template is supplied by thermal energy. Here we present a

model self-replicating system inspired by a class of light switchable colloids and explore the possibility of optimizing the self-replication efficiency (measured by the rate at which templates are replicated) by controlling the frequency at which (light) energy is supplied to the system. Based on extensive computer simulations, we demonstrate that the exponential growth rates of this self-replicating system can be significantly enhanced by delivering the energy pulses at specific frequencies. To the best of our knowledge, this is the first indication that the rate of self-replication can be controlled by the periodicity of external stimuli. The optimization of self-replication does not necessarily require constant energetic expenditure; instead what matters is the proper timing with which the energy is delivered to the system.

4.1 All adaptation is local: Local government capacity and climate change

Emmanuel Nuesiri (enuesiri@illinois.edu)
Geography and Geographic Information Science,
University of Illinois

There is recognition that all adaptation to ecological change is local. However, climate change mitigation and adaptation initiatives very visible at the global level are still insufficient at the local level. This is easily observable on close examination of response mechanisms to various flood events around the world due to extreme weather. In several countries that have experienced massive flooding in recent times, local government authority, the institution mandated to respond to local citizen's needs have lacked the capacity to respond effectively to these flooding events. The consequences have been loss of lives and properties. Using the case study of initiatives to respond to flooding in Cross River State, Nigeria, this presentation shows that local government authorities face severe managerial and technical capacity constraint. These constraints are observed to be related to political will and poor policy planning. The presentation shows that this finding is not limited to Cross River State, but is observed across developed and developing world. The presentation thus makes a call for greater transnational effort to build local government capacity to tackle climate change problems.

4.2 Psychopathology, Adversity, and Creativity: Diversifying Experiences in the Development of Eminent African-Americans

Rodica Damian (ridamian@illinois.edu), Dean Simonton
Department of Psychology, UIUC

Symptoms associated with mental illness were hypothesized to relate to creative achievement because they act as diversifying experiences. However, this theory has only been tested on predominantly majority-culture samples. Do tendencies toward mental illness still predict eminent creativity when they co-exist with other diversifying experiences, such as early parental death, minority-status, or poverty? These alternative diversifying experiences can be collectively referred to as examples of developmental adversity. This conjecture was tested on a significant sample of 291 eminent African-Americans who, by the nature of their status as long-term minorities, would experience more developmental adversity. Replicating majority-culture patterns, African-American artists showed higher mental illness rates than African-American scientists. Yet, the absolute percentages were significantly lower for the African-Americans, regardless of profession. Furthermore, mental illness predicted higher eminence levels only for the African-American artists, an effect that diminished when controlling for developmental adversity. Because the latter predicted eminence for both artists and scientists, the "madness-to-genius" link probably represents just one of several routes by which diversifying experiences can influence eminence. The same developmental ends can be attained by different means.

4.3 They Can Take a Hint: Preserved Integration of Outside Information with Memory in Older Adults

Alex Konkel (agkonkel@wustl.edu), Diana Selmeczy, Ian G. Dobbins
Washington University in St. Louis

Memory ability typically declines with age, leading older adults to rely more on outside sources like lists and caretakers. More generally, memory judgments should be sensitive to contextual cues, including the recommendations of others. Across two experiments we used a cued recognition paradigm to examine how well older adults (compared to college-aged adults) incorporate external cues that forecast the likely old/new status of each recognition test probe. Experiment 1 demonstrated similar cue accuracy benefits for younger and older adults. Experiment 2 confirmed the similar accuracy benefit in older adults across a range of cue validities. Response time analyses suggest that older adults had difficulty reconciling invalid cues with their own memory, although they tend to make the correct decision in the end. Although there was evidence of working memory and executive control decline in our older adult sample, they were nonetheless equally able to integrate external cues into their memory reports, suggesting that judicious weighting of environmental cues was not dependent on either ability and declines minimally if at all with age.

4.4 The role of attentional shifts in graph comprehension

Audrey Michal
(audrey.lustig.michal@northwestern.edu), Steven L. Franconeri
Department of Psychology, Northwestern University

According to one recent account, judging spatial relations (e.g., a small blue bar to the left of a large red bar) is based on ordered attentional shifts. Here we confirm the surprising prediction that the order of attentional shifts has a powerful impact on the direction of the extracted relation, a finding that has direct implications for comprehension of bar graphs. Participants were eyetracked while they made speeded responses to questions of the type "Is the red bar larger than the blue bar?" In an undergraduate population, the more individuals selected the first mentioned (red) bar first, the faster their RTs were (R^2=0.30). In an 8 year-old population, RT was also faster for participants who regularly inspected the first mentioned bar first (R^2=0.41). Surprisingly, more children adopted a strategy of selecting the left bar first, regardless of the question – these participants tended to be slower (R^2=0.32). We observed both optimal (selecting the first mentioned object) and sub-

optimal routines (selecting the left object) for extracting visual relations in graphs, with children showing a greater tendency to attend sub-optimally. The order of attentional shifts accounted for a significant amount of RT variability and thus appears critical for framing 'directionality' of visual relations.

Posters

Poster abstracts are available in the full program on sops.beckman.illinois.edu

5.1 **Yanjing Li** *Transition of Localization Behavior in MoS2 Nanoribbon*

5.2 **Keith Cassidy** *The Bacterial Brain: Looking into a Chemoreceptor Array*

5.3 **Min Kyung Lee** *Colloidal Particle Assembly in Microchanneled, Bioactive Hydrogel for Vascular and Neural Patterning*

5.4 **Canan Dagdeviren** *Conformal Piezoelectric Energy Harvesting and Storage From Motions of the Heart, Lung and Diaphragm*

5.5 **Boon Chong Goh** *Molecular Modeling of the Immature Retroviral Lattice*

5.6 **Jennifer Maier** *The Opossum: A New Model for Intervertebral Disc Development?*

5.7 **Renee Sadowski** *Oral administration of bisphenol A during early development alters adult neuron and glia number in the prefrontal cortex of male, but not female, rats.*

5.8 **Wan-Ting Chen** *Hydrothermal Liquefaction of Mixed-culture Algal Biomass from Wastewater Treatment System into Bio-crude Oil*

5.9 **Kishor Kumar Kalathiparambil** *Erosion effects on tungsten plasma facing components*

5.10 **Hyang Yeon Lee** *Potent and Selective Synergistic Effect of NHI-Glc-2 and DNQ Combination in Cancer Treatment*

5.11 **Mei-Hsiu Lai** *Tailoring Polymersome Bilayer Permeability for Improved Tumor Detection and Imaging*

5.12 **Priya Raman** *Optimized Magnetic Field Configuration for High Power Impulse Magnetron Sputtering*

5.13 **Sumin Kim** *Controlled and Safer Therapeutic Delivery of Venom Peptides using Well-defined Polymeric Nanoparticles for Cancer Inhibition*

5.14 **Santosh Misra** *Nanocelles for Improved Inhibition of Breast Cancer Stem Cells via STAT-3 Cascade Pathway*

5.15 **Aram Yoon** *Understanding oxidation in atomic scale*

5.16 **Dawn Eriksen** *Pathway Engineering through Simultaneous Directed Evolution of Multiple Biosynthetic Pathway Proteins*

5.17 **Bala Mutyala** *Bullying in Illinois Public Schools*

5.18 **Syed Abbas Bukhari** *Socially Responsive Gene Families Are Conserved For Male-Male And Male-Female Social Interactions In Fruit Fly And Stickleback Fish*

5.19 **Sung Jun Lim** *Brightness-equalized quantum dots for quantitative biological imaging*

5.20 **Anabelle Couleau** *Price Volatility Interdependence in the European Biodiesel Industry over and across Markets*

5.21 **Jaime Thissen** *Community-Based Approaches to Addressing Agroecological Integrated Systems in the Brazilian Amazon Rainforest*

5.22 **Aldis Sipolins** *Anodal tDCS during videogame training enhances transfer to the Stroop Effect*

5.23 **Amanda Marciel** *Fluidic-directed assembly of aligned oligopeptides with pi-conjugated cores*

5.24 **Danielle Mai** *Flexible Branched Polymers for Single Molecule Rheology*

5.25 **Daniel Reilly** *Engineering Fluorescent Dendrimer Nanoprobes for Increased Photostability*

5.26 **Laura Mozdzen** *Spatially-graded collagen biomaterials to regenerate the tendon bone junction*

5.27 **Xinxin Feng** *Structures of bacterial diterpene and isoprenoid synthases: Targeting virulence and biofilm formation*

5.28 **Yugang Bai** *Synthesis and application of single-chain polymer nanoparticles*

5.29 **Sayan Bhattacharyya** *Investigating writers' attitudes by mining a large corpus of books*

5.30 **Youhua Tan** *Matrix softness regulates plasticity of tumor-repopulating cells via H3K9 demethylation and Sox2 expression*

5.31 **Santosh Misra** *Regressing Metastatic and Drug Resistant Breast Cancer with Trigger-able Pro-nifuroxasome Nanoparticle by Inhibiting Transcription Factor STAT3*

5.32 **Jun Wu** *α-Catenin cytomechanics: role in cadherin-dependent adhesion and mechanotransduction*

5.33 **Yu-Hsiang (John) Huang** *IT Portfolio Efficient Frontier and Decision Making*

5.34 **Brian Metzger** *Not all probes are created equal: Suppressed-eye probes draw attention to the suppressed eye*

5.35 **Han Xiao** *Exploiting Issatchenkia orientalis SD108 for Succinic Acid Production*

5.36 **Masoud Safdari** *An Isogeometric Interface-enriched Generalized Finite Element Method for Problems with Complex Discontinuous Gradient Field*

5.37 **Jialan Zhang** *Free energy of compositionally graded ferroelectric films*

5.38 **Sara Pedron** *3D hydrogel platforms to study glioblastoma malignancy*

5.39 **Fuzeng Ren** *Self-Organized Nanolayering Induced by Sliding Wear in Cu-Ag two phase alloy*

5.40 **Huijie Lu** *Integrated Meta-Omics: the New Frontier for Environmental Engineering*

5.41 **Kang Mo Ku** *Allelopathic effects of horseradish leaf tissue extract on lettuce seeds*

5.42 **Ivan Shchelkanov** *Contamination particle source in high vacuum deposition systems*

5.43 **Susana Y. Kimura** *Haloacetamide and haloacetonitrile formation from the reaction of Monochloramine and Aldehydes in drinking waters*

5.44 **Natalia Garcia Rey** *The role of CO2 and ionic liquid complex on the electroreduction of carbon dioxide at lower potentials*

Poster Abstracts

5.1 **Transition of Localization Behavior in MoS2 Nanoribbon**

Yanjing Li (li30@illinois.edu), Nadya Mason
Physics Department, University of Illinois

We have measured side-gated nanoribbon in MoS2 at low temperature and observed the transition from coulomb blockade to resonant transmission when tuning Fermi level with the backgate at low temperature. We found at a certain backgate voltage the whole nanoribbon acts as a single quantum dot, which is the transition point for electron to turn from being localized to being delocalized. We also discuss the origin of disorder potential causing the localization.

5.2 **The Bacterial Brain: Looking into a Chemoreceptor Array**

Keith Cassidy (ccassid2@illinois.edu), Juan Perilla, Suvrajit Maji, Peijun Zhang, Klaus Schulten
Physics Department, UIUC

The ability of all living things, from single cells to large multicellular organisms, to sense, interpret, and respond to environmental signals is central to life. Bacteria have

evolved exquisite protein networks, which they use to detect gradients in certain chemicals in their surroundings and alter their swimming behavior. This computation is carried out within the chemoreceptor array, a remarkably ordered supramolecular complex composed of the histidine kinase, CheA; adaptor protein, CheW; and various methyl-accepting chemotaxis proteins (MCPs), which cluster together by the thousands at the cell pole. The clustering of receptors within the chemoreceptor array gives rise to the systems-level information processing properties of bacterial chemotaxis such as signal amplification, ultrasensitivity, and precise adaptation. We present an all-atom structure of a patch of the chemoreceptor array from the thermophile Thermotoga maritima, derived from computational and experimental techniques. The structure suggests a possible molecular mechanism for signal transduction through the array and its functional implications.

5.3 Colloidal Particle Assembly in Microchanneled, Bioactive Hydrogel for Vascular and Neural Patterning

Min Kyung Lee（mklee@illinois.edu, Hyunjoon Kong
University of Illinois at Urbana-Champaign

Controlling spatial organization of growth factor-releasing microparticles in a three dimensional matrix has been long sought to guide the growth direction and spacing of vascular and neural networks; however, it still remains a grand challenge. This study demonstrates that a simple uniaxial freeze drying of a hydrogel loaded with microparticles temporally increase freezing-induced shear stress on and subsequently align microparticles in resulting microchannels. This process with the hydrogel loaded with microparticles releasing vascular endothelial growth factor (VEGF) and also functionalized with cell adhesion peptides resulted in a material that stimulated vascular growth into microchannels and further improved perfusion recovery of ischemic hindlimb. Additionally, coupled with microfabrication, this process assembled a hydrogel that guides neuronal growth exclusively along the microchannels functionalized with cell adhesion peptides. We believe this process would be broadly useful in modifying the microstructure and properties of various hydrogel systems.

5.4 Conformal Piezoelectric Energy Harvesting and Storage From Motions of the Heart, Lung and Diaphragm

Canan Dagdeviren (dagdevi1@illinois.edu), Pauline Joe, Yonggang Huang, Marvin J. Slepian, John A. Rogers
Materials Science and Engineering, University of Illinois

Here, we report advanced materials and devices that enable high efficiency mechanical to electrical energy conversion from the natural contractile and relaxation motion of the heart, lung and diaphragm, demonstrated in several different animal models, each of which has organs with sizes that approach human scales. A co-integrated collection of such energy harvesting elements with rectifiers and microbatteries provides an entire flexible system, capable of viable integration with the beating heart via medical sutures and operation with efficiencies of ~2%. Additional experiments, computational models and results in multilayer configurations capture the key behaviors, illuminate essential design aspects and offer sufficient power outputs for operation of pacemakers, with or without battery assist.

5.5 Molecular Modeling of the Immature Retroviral Lattice

Boon Chong Goh(bcgoh@ks.uiuc.edu), Juan R. Perilla, Katrina J. Heyrana, Rebecca C. Craven, Klaus Schulten
Physics, UIUC

Retroviruses like HIV encode the Group antigen (gag) polyprotein, that contains the matrix protein (MA), capsid protein (CA), nucleo capsid protein (NC), as well as other smaller peptides. Gag is essential during the budding and maturation phases of the virus infective cycle. During assembly of the viral particle gag oligomerizes into a hexameric lattice commonly referred as the immature lattice, in contrast to the mature lattice (virus capsid). Experimental determination, at high-resolution, of the structure of the immature gag lattice has proven to be a challenge for decades. In this work, we present an all-atom model of the immature lattice for the Rous Sarcoma Virus (RSV) based on cryo-electron microscopy and computational modeling. The structural stability of our model is tested through molecular dynamics (MD) simulations. Furthermore, we show that smaller peptides (specifically p10) are critical for the stability of the immature lattice. Additionally, point mutations at the trimeric interface of the lattice result in the production of distorted viral particles and decreased infectivity. Our results suggest that electrostatic interactions at the trimeric interface are essential for the virus assembly and maturation pathways.

5.6 The Opossum: A New Model for Intervertebral Disc Development?

Jennifer Maier (jmaier@illinois.edu), Karen E Sears
Animal Biology, UIUC

The grey short-tailed opossum, (Monodelphis domestica) is a pouchless marsupial. It is currently used to study limb development and evolution. Opossums are born at a premature stage and must climb after birth to the teat in order to complete development. To allow this, the newborns have highly-developed, muscular forelimbs, but the hindlimb's development is delayed. This disparity in limb development led us to ask if the vertebral column, specifically the intervertebral disc (IVD), has delayed development at the hindlimb level. IVDs consist of a central gel-like nucleus pulposus (NP) surrounded by the collagenous annulus fibrosis. Experiments in mice have shown that the NP is the remnant of the embryonic notochord; the annulus is derived from a compartment of the somites. Interestingly, the NP is found only in mammals. The discs are vital to locomotion in vertebrates, and in humans their degeneration during aging can lead to pain and loss of mobility. In the United States, this is a costly ailment with few effective treatments. Understanding how the IVD develops may lead therapies that address disc degeneration. We will characterize the notochord to NP transition of the opossum and compare marsupial and placental disc development at the anatomical and molecular level.

5.7 Oral administration of bisphenol A during early development alters adult neuron and glia number in the prefrontal cortex of male, but not female, rats.

Renee Sadowski (rsadowski82@gmail.com), R.N. Sadowski, L.M. Wise, S.L. Schantz, J.M. Juraska
Beckman Institute, UIUC

Previous work has shown that exposure to bisphenol A (BPA) during early development can alter sexual differentiation of the brain in rodents, although few studies have examined effects on areas of the brain associated with cognition. The current study examined if developmental BPA exposure alters total number of neurons and glia in the medial prefrontal cortex (mPFC) in adulthood. Long-Evans hooded rats were bred in the laboratory, and pregnant rats were orally exposed to corn oil (vehicle), 4 µg/kg, 40 µg/kg, or 400 µg/kg throughout pregnancy. After parturition, pups were given daily oral doses of oil or BPA, corresponding to those given during gestation, from days 1-9. Brains were examined in adulthood (P140), and layers 2/3 and layers 5/6 of the mPFC were parcellated separately to determine volume. The number of neurons and glia in the mPFC were then quantified stereologically with the optical disector. Results indicate that males exposed to 400µg/kg BPA had increased numbers of neurons and glia in layers 5/6. Although there were no significant effects of BPA in layers 2/3, the pattern of increased neuron number in males exposed to 400µg/kg was similar to that seen in layers 5/6. Interestingly, increased neuron number in the PFC has also been reported in autistic male children (Courchesne et al., 2011). No effects of BPA were seen in females or in males exposed to the other doses of BPA. This evidence suggests that males are more susceptible to the long-lasting effects of BPA on the mPFC.

5.8 Hydrothermal Liquefaction of Mixed-culture Algal Biomass from Wastewater Treatment System into Bio-crude Oil

Wan-Ting Chen (wchen58@illinois.edu), Yuanhui Zhang, Jixiang Zhang, Guo Yu, Lance C. Schideman, Peng Zhang,Mitchell Minarick
Agricultural and Biological Engineering, University of Illinois

In this study, a mixed-culture algal biomass harvested from a functioning wastewater treatment system (AW) was hydrothermally converted into bio-crude oils. The highest bio-crude oil yield (49 % of volatile matter) and the highest energy recovery were obtained at 300 °C with 1 hour retention time. The highest heating value of the bio-crude oil was 33.3 MJ/kg, produced at 320 °C and 1 hour retention time. Thermogravimetric analysis showed approximately 60 % of the bio-crude oils were distilled in the range of 200 °C-550 °C; and the solid residue might be suitable for use in asphalt. GC-MS results indicated that the bio-crude oil contained hydrocarbons and fatty acids, while the aqueous product was rich in organic acids and cyclic amines. The nitrogen recovery (NR) in the bio-crude oil ranged from 8.41 % - 16.8 %, which was lower than the typical range of 25 %-53 % from previous studies.

5.9 Erosion effects on tungsten plasma facing components

Kishor Kumar Kalathiparambil (kishor@illinois.edu)
Department of Nuclear, Plasma, and Radiological Engineering, University of Illinois

Erosion of cathode material due to sputtering by ions and fast charge exchange neutrals is a significant consequence of plasma surface interaction in discharge plasmas. The eroded material in the bulk plasma may lead to the formation of nanoparticles by nucleation/agglomeration processes up to micron-sized particles. It is necessary to understand the growth steps since the nanoparticles charging influences the discharge and the macroscopic plasma parameters. Additionally, the presence of dust which materialise as impurities, is a critical problem in processing plasmas and as shown recently, their production in tokamaks could be a drawback for safety reasons. In the present study, the growth of tungsten nanoparticles in sputtering DC discharges is investigated. Argon glow plasmas were created in a parallel electrode configuration with a tungsten disc used as cathode. The operating pressure and the discharge current were kept constant. Dust particles formed in such conditions were collected and analysed using SEM and HRTEM techniques to understand their morphological and structural features. The size distributions were constructed from SEM images. Results indicate that they grow by continuous nucleation and by successive agglomeration processes. The bias voltage, the bulk electron density and the emission intensities of argon and tungsten lines were acquired during the experiments. Their evolution showed distinctive features, explained by a competition between the surface state of the cathode and the nanoparticle growth.

5.10 Potent and Selective Synergistic Effect of NHI-Glc-2 and DNQ Combination in Cancer Treatment

Hyang Yeon Lee (hyanglee@illinois.edu), Paul J. Hergenrother
Chemistry, Institute for Genomic Biology, University of Illinois

Normally, healthy cells primarily use mitochondrial respiration to produce ATP in the presence of oxygen. However tumor cells use aerobic glycolysis known as Warburg effect for energy production even in the presence of oxygen. This distinctive carbohydrate metabolism of tumor cells is one of the important targets to develop anticancer agents. LDHA is an important enzyme that catalyzes conversion of pyruvate into lactate, and over-expressed in many cancer cells by Warburg effect. In this research, we have developed N-hydroxyindole(NHI) derivatives as new LDHA inhibitors. Among them, glucose conjugated NHI, NHI-Glc-2, showed potent anticancer activity by selective inhibition of LDHA and enhanced cellular uptake through over-expressed GLUT1 in cancer cells. Moreover, NHI-Glc-2 was treated with several anticancer agents to evaluate the possibility of combination drug therapy. As a result, DNQ, a NQO1 substrate, was selected as a potent combination pair. Cancer cell death was induced by high synergistic effect of DNQ and NHI-Glc-2 selectively and significantly.

5.11 Tailoring Polymersome Bilayer Permeability for Improved Tumor Detection and Imaging

Mei-Hsiu Lai (lai23@illinois.edu), Sangmin Lee, Cartney E. Smith, Kwangmeyung Kim, and Hyunjoon Kong
Chemical and Biomolecular Engineering, University of Illinois

Nanoparticles formed from intermolecular self-assembly, such as liposomes and polymersomes, are conjugated with various biomedical imaging contrast agents for cancer detection and imaging, taking advantage of the enhanced permeation and retention (EPR) effect. Inadvertently, these nanoparticles undergo fast, dilution-induced disintegration in circulation and quickly lose their capability to associate with and image cancerous sites. To resolve this challenge, we hypothesize that polymersomes with low permeability of the bilayer allow us to extend their lifetime in circulation and improve the quality of cancer detection and imaging. This hypothesis is examined by using a polymersome of poly(2-hydroxyethyl-co-octadecyl aspartamide) (PHEA-C18) as a model nanoparticle. The PHEA-C18 is sequentially modified with methacrylate groups. The bilayer permeability of polymersomes is tailored by increasing the packing density of the bilayer with hydrophobic methacrylate groups and further cross-linking them. The resulting polymersome demonstrates greater stability in physiological media both at physiological and elevated temperatures than the polymersome free of methacrylate groups. Ultimately, the polymersome with cross-linked bilayer and labeled with a near-infrared (NIR) fluorescent dye is able to sustainably highlight squamous cell carcinoma tumors in mice over two days. We envisage that the resulting nanoparticles will not only improve cancer diagnosis but also further image-guided therapies.

5.12 Optimized Magnetic Field Configuration for High Power Impulse Magnetron Sputtering

Priya Raman (raman6@illinois.edu), Ivan Schelkano, David Neil Ruzic
Department of Nuclear Plasma and Radiological Engineering, UIUC

Magnetic field design is critical in magnetron sputtering systems at it affects the plasma parameters and film quality. Most magnetic field configurations are designed for DC sputtering and they suffer from low target utilization, non-uniform ionized metal atoms, etc. High Power Pulsed Magnetron Sputtering (HPPMS) discharge has high degree of ionization of the sputtered material with very high peak power on the target. It has been confirmed from our work on HPPMS that a spiral-shaped magnetic field design on 36 cm diameter copper target was able to produce superior plasma uniformity on the substrate in addition to improved target utilization without the need for magnet rotation. Commercial 10cm (4 inch) diameter magnetrons are very popular and they have a circular magnetic field design. To optimize the magnet field configuration in HPPMS for the 4 inch (10cm) cathode gun, the spiral design from the 36mm target was scaled down and modified to produces the same magnetic field magnitude and race track pattern on the 4 inch target surface. Various COMSOL software simulations were done to achieve better electron trapping efficiency in the 4 inch cathode gun magnetron design for HPPMS.

5.13 Controlled and Safer Therapeutic Delivery of Venom Peptides using Well-defined Polymeric Nanoparticles for Cancer Inhibition

Sumin Kim (kim418@illinois.edu), Santosh Kumar Misra, Dipanjan Pan
University of Illinois, Carle

Myriad of advancement has been made to identify naturally abundant substances for use as therapeutic agents. Host defence peptides (eukaryotic cells) from animal venoms have been identified to possess substantial anticancer properties. However, their therapeutic potential cannot be fully realized without a controlled delivery mechanism because of off-target toxicity, non-specificity, complement activation issues and unfavorable pharmacokinetics, all contributed to a failed phase I clinical trial. Towards a safer, translatable approach, we have developed a viable chemical methodology based on well-defined, self-assembled polymeric nano-architecture for controlled delivery of venom peptides.

Although our methodology is applicable for peptides of 5-30 aa, as a specific example, Melittin, a well-studied cytolytic peptide, was selected for preliminary studies. The parent nanoparticles were self-assembled as aqueous suspension of amphiphilic diblock-co-polymer PS-b-PAA and Polyoxyethylene (20) cetyl ether (70±5 nm) and loaded with melittin by a post-incubation methodology. These particles showed remarkable stability over time and the release of melittin is well controlled in time and concentration dependent way. The cytotoxicity of these nanoparticles was studied in MCF-7 and MDA-MB231 breast cancer cells using MTT assay. This construct promises to address the serious off-target toxicity of the membrane-bound venom peptides when systemically delivered and simultaneously protects the integrity of the peptide itself that may complicate systemic application. The synthesis, characterization, shelf-serum stability and biological evaluation will be discussed.

5.14 Nanocelles for Improved Inhibition of Breast Cancer Stem Cells via STAT-3 Cascade Pathway

Santosh Misra (skmisra@illinois.edu), Dipanjan Pan
Deptartment of Bioengineering, UIUC

The root cause of low survival rate in breast cancer patients is the resistance to conventional therapies and recurrence of the disease because of unaffected stem like cells after chemotherapy. Cancer stem cells are reported to be controlled by pathways that are dormant in normal adult cells, e.g. PTEN, which is a negative regulator of transcription factor STAT3. STAT3 regulates genes that are involved in stem cell self-renewal and thus represents a novel therapeutic target of significant clinical importance. Herein we describe for the first time a novel therapeutic strategy to target breast cancer stem-like cells via STAT-3 inhibition and provide encompassing to chemotherapeutic agent for efficient delivery. We have developed self-assembled nanoparticle from amphiphilic PS-b-PAA and brij58 (nanocelles). Solvent evaporation method was used to generate particles with and without niclosamide, a well-studied STAT3 inhibitor. Hydrodynamic diameter of the nanocelle particles (95±5) was significantly different from blank nanoparticles (70±5). Nanocelles were further evaluated for their cytotoxicity studies using Trypan Blue and MTT assay in MDA-MB231 and MCF-7 cells.

Nanocelles were at least 4 fold better in inhibiting breast cancer cell growth compared to niclosamide. This presentation will disclose the physico-chemical characterization of the nanoparticles, their cellular assays and further bio-studies to confirm abolition of stem cell-subpopulation.

5.15 Understanding oxidation in atomic scale

Aram Yoon (ayoon5@illinois.edu), Jian-Min ZuO
Materials Science and Engineering, University of Illinois

In small world, oxidation becomes an important phenomenon. For example, if you make a 10 nm nanoparticle of iron, 1 or 2 nm of the surface will be rapidly and spontaneously oxidized into iron oxide, which means that 10~20 % of the matter is not what you intended. Also, oxidation can change the entire shape of the nanostructure making voids in it (Kirkendall effect), resulting in unexpected structure and properties. Therefore, utilizing nanostructure would be more demanding without consideration of oxidation. One of the purely understood phenomena in oxidation is its early stage which occurs so fast that it was hard to observe so far. We have shown the early stage of oxidation of iron nanoparticles by in-situ transmission electron microscope study. We discuss its dynamic changes and dependence on the structural factors of the nanoparticles.

5.16 Pathway Engineering through Simultaneous Directed Evolution of Multiple Biosynthetic Pathway Proteins

Dawn Eriksen (eriksen1@uiuc.edu), Pei Chiun Helen Hsieh, Patrick Lynn, Huimin Zhao
Energy Biosciences Institute, UIUC

The optimization of metabolic pathways is critical for efficient and economical production of biofuels and specialty chemicals. One significant pathway important for optimization is the cellobiose utilization pathway, identified as a promising route in biomass utilization. Here we describe the optimization of cellobiose consumption and ethanol productivity by simultaneously engineering both proteins of the pathway, the β-glucosidase (gh1-1) and the cellodextrin transporter (cdt-1), in an example of pathway engineering through directed evolution. The improved pathway was assessed based on the strain specific growth rate on cellobiose, with the final mutant exhibiting a 47% increase over the wild-type pathway. Metabolite analysis of the engineered pathway identified a 49% increase in cellobiose consumption and a 64% increase in ethanol productivity. By simultaneously engineering multiple proteins in the pathway, the overall flux of the pathway and protein activity were balanced, allowing for optimal pathway performance. This optimization can be generally applied to other metabolic pathways, provided a selection/screening method is available for the desired phenotype. This improved in vivo cellobiose utilization could help to decrease the in vitro enzyme load of biomass pretreatment, ultimately contributing to a reduction in the high cost of biofuel process economics.

5.17 Bullying in Illinois Public Schools

Bala Mutyala (Mutyala2@illinois.edu)
Center for Prevention Research and Development, University of Illinois

Bullying in schools is an important public health problem that is threatening the physical and mental wellbeing of students. To identify factors responsible for school bullying in Illinois, a cross-sectional study was conducted with the 2012 Illinois Youth Survey data. Logistic regression was performed accounting for multistage sampling design and weighting. During 2012, 37.77% (n=3662) of students from 130 Illinois public schools reported multiple forms of bullying such as name calling, threatening, hitting and cyberbullying. Whites, females, victims of dating abuse, students with depression, suicidal thoughts, and those who were dissatisfied and felt unsafe at school had higher odds of reporting past year bullying, after adjusting for other covariates. Students from rural and other urban/suburban (non-Chicagoland) public schools had higher odds of bullying than those from Chicago. Whereas, the odds of reporting past year bullying decreased with increasing age, selling illegal drugs at school and non-participation in school/community activities in the past year among Illinois public school students. Bullying prevention programs and policies in Illinois public schools require comprehensive action ranging from creating a positive school climate, clear and well enforced anti-bullying policies, and early identification and support for victims as well as perpetrators.

5.18 Socially Responsive Gene Families Are Conserved For Male-Male And Male-Female Social Interactions In Fruit Fly And Stickleback Fish

Syed Abbas Bukhari (sbukhar@illinois.edu), Alison M. Bell
Ilinois Informatics Institute (I3), University of Illinois

There is growing evidence that social interactions elicit changes in brain gene expression. However, we know little about whether the same molecular processes are associated with similar behavioral responses in different species. One tactic for understanding the evolution of social behavior is to quantify genomic responses to social stimuli in different species and mine for conserved genomic elements. Here we test the hypotheses that there are conserved sets of gene families that are responsive to social interactions in Gasterosteus aculeatus (sticklebacks) and Drosophila melanogaster (fruit fly). Brain gene expression was quantified in male sticklebacks in response to a territorial challenge by another male or in response to a courtship opportunity with a female stickleback (control: no stimulus). Socially responsive genes underlying males' responses to a territorial challenge by another male and to a mating opportunity with a female in Drosophila were extracted from Ellis et al (2011). Both fish and fly socially responsive genes sets were assigned PANTHER Families using PANTHER HMM Assignments. To identify shared transcription factors binding sites in PANTHER families, 5kb gene upstream sequences were searched for known insect TRANSFAC motifs via TFM-Explorer. We found 3 PANTHER genes families that were responsive to a territorial challenge in both Drosophila and Sticklebacks, and 27 gene families that were responsive to a courtship opportunity in both species. Shared gene families include genes for novel transcription factors, receptor activity and enzyme activities such as methyltransferases, protein kinases, GTPases, metallopeptidases, phosphorylases and oxidoreductases. Interestingly, most genes within

PANTHER families also shared binding sites for one or more transcription factors. These results suggest that some neurogenomic responses to social stimuli are conserved across distantly-related species, and suggest that commonalities might occur at a higher level, e.g. gene families, rather than at the level of individual genes.

5.19 Brightness-equalized quantum dots for quantitative biological imaging

Sung Jun Lim (melsj@illinois.edu), Mohammed Zahid, Andrew M. Smith
Bioengineering, UIUC

Due to their bright, stable, and color-tunable fluorescence, Quantum dots (QDs) are becoming a powerful tool for highly sensitive multiplexed fluorescent imaging in biomedical researches. However, conventional QDs with different fluorescent colors suffer large brightness disparity that are not ideal for quantitative imaging applications. Here, we introduce a set of novel "brightness-equalized" QDs that are showing various visible colors with same brightnesses.

5.20 Price Volatility Interdependence in the European Biodiesel Industry over and across Markets

Anabelle Couleau (couleau2@illinois.edu), David Laborde

While ethanol is mainly produced by the United States (US) and Brazil, the European Union (EU) dominates world biodiesel production. European biodiesel forms a significant part of the world biodiesel market, about 52% of world production based on average 2008 and 2010 volumes. Although the US biofuel sectors has been largely studied in co-movement in volatility dynamics, what is the volatility dynamics behavior of biofuel related markets in the EU? Our objectives are twofold: (1) assessing price volatility interdependence in the European biodiesel industry over time and across markets, (2) identifying impacts of policy external shocks on those markets. Our analysis aims to evaluate price volatility interdependence in the European biodiesel industry over time and across markets by using a Multivariate Generalized AutoRegressive Conditional Heteroscedastic (MGARCH) model. It thus allows to consider both together the responses of both food price levels and volatility to unanticipated shocks. We then applied a parametric approach using a trivariate VAR-DCC model (Vector AutoRegressive and Dynamic Conditional Correlation) to three markets: crude oil, biodiesel and rapeseed oil during the 2007-2013 period and weekly sport prices. Robustness analyses were conducted to suggest the sensibility of results to future versus spot prices.

5.21 Community-Based Approaches to Addressing Agroecological Integrated Systems in the Brazilian Amazon Rainforest

Jaime Thissen (thissen2@illinois.edu), Kathryn Solorzano Lowell, Lakiah Clark, Vanessa Rivera Quiñones
UIUC

Conventional and modern agriculture faces a number of problems including pollution, land degradation, and the depletion of groundwater. The causes of these environmental crises are rooted in prevalent socio-economic structures that do not account for complex interactions within an ecosystem. The current deforestation of the Brazilian Amazon rainforest is a reflection of these issues. Certain approaches towards social and agricultural development have decreased biodiversity and threatened the lives of indigenous people. Agroecology is an ecological approach to agriculture production that considers interactions between humans, resources and the environment. It serves as an alternative approach to conventional agriculture as a response to current environmental and social problems. The purpose of this study was to assess the effectiveness of current practices in agroecological research. We accomplished this by finding and evaluating sustainable, methodological approaches of these practices in the Brazilian Amazon rainforest. We examined processes of experimental design, the analysis of integrated systems, and the implementation of community education in conservation. Initial results from a literature review on sustainability in the Brazilian Amazon rainforest revealed lacking sustainable development and non-holistic analyses. Future work involves modeling of decision-makers and stakeholders modeling for sustainable development focusing on food security within the Brazilian Amazon rainforest.

5.22 Anodal tDCS during videogame training enhances transfer to the Stroop Effect

Aldis Sipolins (aldis.sipolins@gmail.com), Arthur Kramer
Visual Cognition & Human Performance, Beckman Institute, UIUC

tDCS shows great promise as an adjunct to cognitive training by reliably improving 'online' task performance (i.e., during stimulation). It remains unclear, however, whether tDCS can influence transfer to non-trained tasks (Martin et al., 2013). My project investigated the effects of tDCS administered during videogame training on both online performance and transfer. 45 subjects completed ten 1-hour training sessions with the Space Fortress videogame, a complex and difficult game. Subjects were randomized to receive 2.0 mA of anodal, cathodal, or sham stimulation to the left dorsolateral prefrontal cortex (LDLPFC – F3 in the 10/20 system) for 15 minutes at the start of each training session. Participants who received anodal tDCS during training showed a lower Stroop Effect at post-training compared to cathodal and sham groups. Such effects are consistent with the role of the LDLPFC in executive function generally and the Stroop task specifically (Vanderhasselt, De Raedt, & Baeken, 2009). A lower Stroop effect indicates an improvement in executive function and is especially remarkable given that online Stroop performance is unaffected by tDCS administered to the LDLPFC (Fecteau et al., 2007). Enhancing transfer to a functionally relevant task lends strong support to the usefulness of tDCS in videogame-based cognitive training.

5.23 Fluidic-directed assembly of aligned oligopeptides with pi-conjugated cores

Amanda Marciel (marciel1@illinois.edu), Melikhan Tanyeri, Brian D. Wall, John D. Tovar, William L. Wilson, and Charles M. Schroeder
Biophysics, University of Illinois

In this work, we report the fluidic-directed assembly of aligned pi-conjugated oligopeptides using a tailored laminar

flow called planar extenional flow. Prior methods for fluidic-directed assembly have mainly relied on laminar co-flowing streams with uniform fluid velocities, which precludes fine-scale control required for nanostructure alignment. Here, we capitalize on planar extensional flow to induce alignment of underlying material suprastructures due to a dominant extensional/compressional character for this flow type. We demonstrate that our microfluidic-based method enables reproducible 'triggering' of assembly, along with reliable formation of aligned hierarchical constructs that do not form spontaneously in solution. In this way, fluidic-directed assembly of supramolecular structures allows for unprecedented manipulation at the nano- and mesoscale, which provides rapid and efficient control of electronic or optoelectronic materials properties.

5.24 Flexible Branched Polymers for Single Molecule Rheology

Danielle Mai (djmai2@illinois.edu), Amanda B. Marciel, Christopher A. Brockman, Charles M. Schroeder
Chemical and Biomolecular Engineering, UIUC

We report the synthesis and characterization of branched biopolymers for single molecule rheology. In our work, we utilize a hybrid enzymatic-synthetic approach to graft DNA branches to DNA backbones, thereby producing branched polymers with three arm star, H-shaped, or macromolecular comb-like architectures. The branches and backbones are synthesized via polymerase chain reaction with chemically modified deoxyribonucleotides (dNTPs): branches consist of a terminal azide group, and backbones contain dibenzylcyclooctyne-modified (DBCO) dNTPs. In this way, we utilize strain-promoted, copper-free cycloaddition "click" reactions for facile grafting of azide-terminated branches at DBCO sites along backbones. Copper-free click reactions are bio-orthogonal and nearly quantitative when carried out under mild conditions. We characterized these materials using gel electrophoresis, HPLC, and MALDI-MS, and our branched materials are suitable to study at the single-molecule level. In future work, we will utilize a microfluidic-based hydrodynamic trap to observe branched polymer behavior under various flow conditions. Overall, we seek a molecular-based understanding of the non-equilibrium dynamics of polymer chains, which is crucial for control in processing and molecular self-assembly.

5.25 Engineering Fluorescent Dendrimer Nanoprobes for Increased Photostability

Daniel Reilly (dreilly2@illinois.edu), Sung Hoon Kim, John A. Katzenellenbogen, Charles M. Schroeder
Department of Chemical and Biomolecular Engineering, UIUC

Recent advances in fluorescence microscopy have enabled improvements in spatial resolution for biological imaging. However, there is a strong need for development of advanced fluorescent probes to enable a molecular-scale understanding of biological events. In this work, we report the development of a new class of probes for fluorescence imaging based on dye-conjugated dendrimer nanoconjugates. We utilize molecular-scale dendritic scaffolds as fluorescent probes, thereby enabling conjugation of multiple dyes and linkers to the scaffold periphery. In particular, we use polyamidoamine dendrimers as molecular scaffolds, wherein dye conjugation can be varied over a wide range. Single molecule fluorescence imaging shows that dendrimer nanoconjugates are far brighter than single fluorophores, resulting in increased localization precision. In addition, we further developed a new set of remarkably photostable probes by conjugating photoprotective triplet state quenchers directly onto the dendritic scaffold. We observe large increases in the photobleaching times compared to single dyes and reduced transient dark states (blinking). Overall, we believe that these new probes will allow for single molecule imaging over long time scales, enabling new vistas in biological imaging.

5.26 Spatially-graded collagen biomaterials to regenerate the tendon bone junction

Laura Mozdzen (mozdzen2@illinois.edu), Michelle Oyen, Hazel Screen, Brendan Harley
Chemical and Biomolecular Engineering, University of Illinois

The tendon bone junction (TBJ) is a unique anatomical zone containing local structural and mechanical gradients that transmit loads between tendon and bone. TBJ injuries such as rotator cuff tears are common, with >4.5 million physician visits and 250,000 surgeries nationally each year. Current surgical approaches are unable to regenerate the TBJ, leading to extremely high (>90%) re-failure rates in some cases. My project focuses on developing a collagen-glycosaminoglycan (CG) scaffold which mimics elements of the biophysical and biochemical heterogeneities of the native TBJ. Our goal is to induce spatially-selective mesenchymal stem cell (MSC) differentiation as a precursor to generating a material to improve biological fixation between tendon and bone. Physical stress concentrations across the TBJ interface impact device mechanical competence. We are employing biomimetic geometries found in the plates of turtle shells and in armored fish to create single CG biomaterials containing distinct non-mineralized and mineralized compartments that display improved tensile competence. We can characterize cellular microenvironments across the interface and have also demonstrated that cells respond differently to strain depending on what materials they are interacting with. Our aim is to generate prototype CG scaffolds with improved mechanical and bioactive properties to aid regenerative repair of the TBJ.

5.27 Structures of bacterial diterpene and isoprenoid synthases: Targeting virulence and biofilm formation

Xinxin Feng (feng21@illinois.edu), Wei Zhu, Yi-Liang Liu, Kai Li, Eric Oldfield
Department of Chemistry, University of Illinois

We report the X-ray structures of two bacterial terpene synthases: tuberculosinol/(13R,S)-iso-tuberculosinol synthase (Rv3378c) from Mycobacterium tuberculosis, involved in virulence factor formation, and YisP from Bacillus subtilis, involved in biofilm formation. Both enzymes contain the DDXXD domains found in most enzymes in terpene biosynthesis and act on terpene diphosphate substrates. Rv3378c acts as a phosphatase and its structure is unique for a terpene synthase, closely resembling that of the cis-isoprenoid diphosphate synthases involved in bacterial cell wall biosynthesis. We solved structures with bound substrates and an inhibitor

and these results combined with site-directed mutagenesis lead to a mechanism of action in which two Tyr residues activate water molecules for nucleophilic attack on the tuberculosinol diphosphate substrate. The BsYisP structure closely resembles that of dehydrosqualene synthase (CrtM, used in formation of the S. aureus virulence factor staphyloxanthin), but it also acts as a phosphatase and produces farnesol. We show that both tuberculosinol and farnesol affect membrane structure in a cholesterol-like manner that may be associated with their effects on virulence or biofilm formation. The results are of broad general interest in the context of mechanistic enzymology as well as in drug discovery in which membrane structure modulators are targeted.

5.28 Synthesis and application of single-chain polymer nanoparticles

Yugang Bai (bai11@illinois.edu), Hang Xing, Gretchen A. Vincil, N. Gabriel Lemcoff, Yi Lu and Steven C. Zimmerman
Department of Chemistry, University of Illinois

Linear polymer from ring-opening metathesis polymerization can be facilely and efficiently functionalized by allyl groups, and intramolecularly crosslinked by ring-closing matethesis to yield single-chain polymer particles controllably with valency control. The particles serve as excellent carriers as functionalities of interest can be loaded in any stage during synthesis, and the particles themselves can be tuned water-soluble through dihydroxylation. Wide application of such particles can be anticipated. For example, the particles showed to be excellent protective carriers for unstable fluorophores such as Fluorescein. Aminated particles showed capability of gene delivery. Dihydroxylated particles can serve as templates for metal nanoparticle formation. We are still actively searching for the capabilities of this material in light harvesting and antimicrobial fields.

5.29 Investigating writers' attitudes by mining a large corpus of books

Sayan Bhattacharyya (sayan@illinois.edu), Rini Bhattacharya Mehta
Graduate School of Library and Information Science, Program in Comparative and World Literature ,UIUC

Researchers in history or literary studies are often interested in the question of attitudes of writers to some specific subject matter, and seek an efficient discovery mechanism that can identify which texts in a large collection of texts would repay close study for the purpose of exploring this question. Our work-in-progress approaches this problem in a scalable way by combining a search for collocations within the corpus using a list-based approach, with filtering using available bibliographic metadata. Our use case involves investigating the attitudes of French-language and English-language writers towards women's work in the colonized world. Our approach is to generate separate lists of occurrences (indexed by line number, page number, and book id number) of all occurrences of words relating to womanhood (and a set of close synonyms), of all occurrences of words relating to work (and a set of close synonyms), and of all occurrences of words expressive of attitudes. We then identify, based on these separate lists, instances of co-occurrences of all three items within a determinate proximity window. This list of co-occurrences serves as the basis for the discovery mechanism for identification of relevant texts, as well as for aggregate-level analysis enabling comparative measures.

5.30 Matrix softness regulates plasticity of tumor-repopulating cells via H3K9 demethylation and Sox2 expression

Youhua Tan (yhtan@illinois.edu), Arash Tajik, Junwei Chen, Ning Wang
Mechanical Science and Engineering, University of Illinois

Tumor-repopulating cells (TRCs) are a self-renewing, tumorigenic subpopulation of cancer cells critical in cancer progression. However, the underlying mechanisms of how TRCs maintain their self-renewing capability remain elusive. Here we show that melanoma TRCs are progenitor cells of melanocytes. In contrast to differentiated melanoma cells, TRCs had a low level of histone 3 lysine residue 9 (H3K9) methylation that was unresponsive to matrix stiffness or applied forces. After re-plated back to rigid substrates, TRCs exhibited plasticity in Cdc42-mediated mechanical stiffening, H3K9 methylation, Sox2 expression, and self-renewal capability. Differentiated melanoma cells elevated their self-renewal capability in a Sox2-dependent manner when H3K9 methyltransferase G9a or SUV39h1 was silenced. Methylated H3K9 specifically bound Sox2 promoter region to inhibit Sox2 expression that was essential in maintaining self-renewal and tumorigenecity of TRCs both in vitro and in vivo. TRC growth could be greatly inhibited by differentiation or stiff matrices. Taken together, our data suggest that soft–fibrin-matrix-mediated cell softening, H3K9 demethylation, and Sox2 gene expression are essential in regulating TRC self-renewal.

5.31 Regressing Metastatic and Drug Resistant Breast Cancer with Trigger-able Pro-nifuroxasome Nanoparticle by Inhibiting Transcription Factor STAT3

Santosh Misra (skmisra@illinois.edu), Mao Ye, Dipanjan Pan
Department of Bioengineering, UIUC

Cancer chemotherapy is judged effective when it reduces tumor burden by blocking the proliferation and inducing apoptosis of cancer cells. In practice, often it recurs or metastasizes shortly after the primary tumor has been exterminated. Cancer stem cells are reported to be controlled by pathways that are dormant in normal adult cells, e.g. PTEN, which is a negative regulator of transcription factor STAT3. STAT3 regulates genes that are involved in stem cell self-renewal and thus represents a novel therapeutic target of significant clinical importance.
This work, for the first time, reports a nanomedicine-strategy for selective and safer delivery of STAT3 inhibitors for metastatic and drug resistant breast cancer. We have synthesized a novel lipase-labile SN-2 phospholipids-pro-drug from a clinically investigated inhibitor, nifuroxazide, which is regioselectively cleaved by the membrane abundant enzymes in cancer cells. Pro-nifuroxazide was used to formulate the nanoparticles (Pro-nifuroxasome) and the cytotoxic ability of pro-nifuroxasomes (80±5nm) was screened in ER(+)-MCF-7 and ER(-)-MD-MB231 cells at 48h-72h using MTT proliferation assay. Results indicated that pro-nifuroxasomes are fivefold more effective towards

inhibiting ER(+)-MCF-7-cells in a time dependent manner compared to nifuroxazide. This talk will disclose the physico-chemical characterization of the nanoparticles, their cellular assays and further bio-studies to confirm abolition of stem cell-subpopulation.

5.32 α-Catenin cytomechanics: role in cadherin-dependent adhesion and mechanotransduction

Jun Wu (junwu5755@gmail.com), Adrienne K. Barry, Ismaeel Muhamed, Hamid Tabdili, Nitesh Shashikanth, Guillermo A. Gomez, Alpha S. Yap, Cara J. Gottardi, Johan de Rooij, Ning Wang, and Deborah E. Leckband
Chemical and Biomolecular Engineering, UIUC

Cadherins are calcium dependent transmembrane glycoproteins. They are major components of cell-cell adhesion junctions involved in tissue development and organization. Cadherins have been identified as a mechanosensor. The cadherin mechanosensing involves α-catenin. In our study, we demonstrate the role of α-catenin in cadherin-based adhesion and mechanotransduction, in different mechanical contexts. Bead-twisting measurements in conjunction with imaging, and the use of different cell lines and α-catenin mutants reveal that the acute, local mechanical manipulation of cadherin bonds triggers vinculin and actin recruitment to cadherin adhesions, in an actin- and α-catenin-dependent manner. The modest effect of α-catenin on two-dimensional binding affinities of cell surface cadherins further suggests that force-activated adhesion strengthening is due to enhanced cadherin/cytoskeletal interactions rather than to α-catenin-dependent affinity modulation. Complementary investigations of cadherin-based rigidity sensing also suggest that, although α-catenin alters traction force generation, it is not the sole regulator of cell contractility on compliant, cadherin-coated substrata.

5.33 IT Portfolio Efficient Frontier and Decision Making

Yu-Hsiang (John) Huang (huang150@illinois.edu), Yu-Ju (Tony) Tu and Michael J. Shaw
Department of Business Administration, UIUC

Many enterprise executives frequently cope with the challenge of making appropriate IT investment decisions under conditions of uncertainty. Therefore, we propose a highly effective approach − IT Portfolio Efficient Frontier for improving the efficiency in the allocation of IT investment. Moreover, our methodology is based on mathematical optimization, computational experiment, and simulated data. We found that IT Portfolio Efficient Frontier can be applied to a variety of IT project portfolios within a firm, since our proposed approach incorporates the characteristics of Markowitz Portfolio Theory (MPT)-based portfolio model and Data Envelopment Analysis (DEA)-based project selection model. In line with this perspective, the aim of this research is to enable a firm to select the optimal IT portfolio that meets multiple heterogeneous investment objectives, thus making significant contributions to both academic and business communities. Keywords: IT Portfolio Efficient Frontier, Decision Making, Markowitz Portfolio Theory (MPT), Data Envelopment Analysis (DEA)

5.34 Not all probes are created equal: Suppressed-eye probes draw attention to the suppressed eye

Brian Metzger (bmetzge2@illinois.edu), Kyle Mathewson, Evelina Tapia, Kathy Low, Ed Maclin, Monica Fabiani, Gabriele Gratton, Diane Beck
Department of Psychology, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign

Binocular rivalry occurs when disparate images are shown simultaneously but separately to each eye. Perceptually dominant images reverse over time, with one image temporarily dominating perception while the other is suppressed. Probes presented to the suppressed eye are typically seen by participants and tend to cause perception to shift to the suppressed image. Here we ask why perception shifts to the suppressed eye. One possibility is that the probe draws attention to the suppressed eye/image. Prior fMRI research has implicated regions of the dorsal attention network in binocularly rivalry reversals more generally, and EEG research has shown specifically that suppressed-eye probes presented during binocular rivalry elicit larger ERP P3 responses, which have been associated with attentional orienting and allocation, compared to dominant-eye probes. We combine behavior, EEG, and fast event-related optical imaging (EROS) to test the hypothesis that suppressed-eye probes are eliciting a shift in attention to the suppressed image. We find enhanced ERP N2 amplitude, which is thought to index attentional processing, followed by enhanced P3 amplitude for suppressed-eye probes compared to dominant-eye probes. Most notably, greater single-trial P3 amplitude evoked by suppressed-eye probes was correlated with faster subsequent switches to the suppressed image, suggesting the P3 may play a critical role in the switch. Furthermore, EROS data show greater activity for suppressed-eye probes compared to dominant eye-probes occurring in visual cortex and right intraparietal sulcus starting around 400 ms. followed by greater activity in right dorsolateral pre-frontal cortex starting around 700 ms., all of which occurs before the subsequent switch is complete. These later regions belong to the dorsal attention network, thus again implicating attention in the switch. Together, the behavioral, ERP, and EROS data indicate suppressed-eye probes are followed by classic neural markers of attention which may be critical to eliciting a reversal to the suppressed image.

5.35 Exploiting Issatchenkia orientalis SD108 for Succinic Acid Production

Han Xiao (hanxiao@illinois.edu), Zengyi Shao, Yu Jiang, Sudhanshu Dole and Huimin Zhao
Department of Chemical and Biomolecular Engineering, University of Illinois

The toxicity of organic acids presents a key challenge to the development of an economically viable fermentation process for organic acids production. Here we report the discovery, characterization, and engineering of a yeast strain, Issatchenkia orientalis SD108, that is tolerant to low pH and high concentration of organic acids. This strain demonstrated a higher tolerance compared to I. orientalis ATCC 24210 and Classic Distiller's Turbo yeast. In order to explore SD108 as a potential platform organism for organic acid production, we determined its draft genome sequence

and use the sequencing information to guide pathway design. As proof of concept, an engineered four-gene expression cassette related to the reductive TCA cycle was assembled and integrated into the genome of a uracil auxotroph of SD108. The resulting strain was able to produce succinic acid with a titer of 11.63 g/L, yield of 0.12 g/g, and productivity of 0.11 g/L•h in batch cultures using shake flasks.

5.36 An Isogeometric Interface-enriched Generalized Finite Element Method for Problems with Complex Discontinuous Gradient Field

Masoud Safdari (msafdari@illinois.edu), Philippe H. Geubelle, Nancy R. Sottos
Aerospace Engineering Department, University of Illinois

An Isogeometric Interface-enriched Generalized Finite Element Method (IIGFEM) is developed to analyze problems with complex, discontinuous gradient fields commonly observed in the structural, thermal and multiphysics analysis of heterogeneous materials. In problems with high geometrical complexity, the creation of regular (conforming) finite element meshes often represents a significant amount of the analysis time. In the proposed approach, the mesh generation burden is significantly reduced by utilizing simple structured meshes that do not conform to the complex microstructure of the heterogeneous media. Non-Uniform Rational B-Splines (NURBS), commonly used in computer aided design (CAD), are adopted in the IIGFEM to augment the finite element approximation space and capture the weak discontinuity present along material interfaces. IIGFEM utilizes a NURBS basis to represent the geometry, solution field and enrichment functions. Beyond the ability to model complex interfaces, the IIGFEM offers other advantages, such as the simplicity and accuracy of numerical integration, the straightforward implementation of essential boundary conditions, and the flexibility in the choice of the local solution refinement. The convergence, accuracy and stability of the IIGFEM in solving elasto-static problems are studied and compared to the standard finite element method. It is observed that the IIGFEM provides a more precise solution with an optimal rate of convergence.

5.37 Free energy of compositionally graded ferroelectric films

Jialan Zhang (jzuiuc@illinois.edu), Lane Martin
Materials science & engineering, University of Illinois

Ferroelectric thin films are attractive candidates for portable dielectric and electro-thermal device applications due to their low cost, low power consumption, and a wide operating range of temperature. In recent years, graded ferroelectrics have received a great deal of interest as they exhibit behavior and properties that are not observed in their homogenous counterparts. Barium strontium titanate (BaxSi1-xTiO3, BST) thin films are excellent perovskite ferroelectric material system in tunable microwave telecommunication devices due to their high dielectric response. Their pyroelectric properties can be employed in sensors in intruder alarms, fire detection, environmental monitoring, gas analysis, radiometers, laser detectors, uncooled thermal imaging, and in solid-state cooling devices. Here we use a nonlinear thermodynamic model based on Landau-Ginzburg-Devonshire formalism to describe the free energy in compositionally graded BaTiO3-BST ferroelectric films by considering free energy from the following three factors: flexoelectricity, composition gradient, and depolarization field. By taking into account the appropriate mechanical boundary conditions and the commensurate electrostrictive coupling of in-plane misfit strain and polarization, we provide a quantitative computational analysis for the effect of these three energies and their relative magnitude on the ferroelectricity, pyroelectric response and dielectric permittivity in graded BST-BTO films at different temperatures on GdScO3 substrate.

5.38 3D hydrogel platforms to study glioblastoma malignancy

Sara Pedron (spedron@illinois.edu), Eftalda Becka, Brendan Harley
Institute for Genomic Biology, University of Illinois

Human glioblastoma multiforme (hGBM) is a common and very aggressive form of primary brain tumor. Platforms to replicate the tumor microenvironment are a critical topic in the field of cancer research. These technologies can integrate the heterogeneity of glioma and serve as diagnostic platforms for clinical assessment of therapeutic strategies. We have developed a versatile gelatin-based biomaterial scaffold to present combinations of mechanical, structural, and cellular cues inspired by the native glioblastoma microenvironment. Strategies to decorate these biomaterials with biomolecular cues (e.g. hyaluronic acid) and common glioma mutations (e.g. EGFR) demonstrate an impact in their response to microenvironment. Moreover, spatial and temporal gradients regulate the cell proliferation, migration, and differentiation during cancer. Hydrogels containing HA show significant impact on GBM malignancy metrics in comparison to 2D culture or through the use of 3D GelMA or PEGDA hydrogels. Using this tool we aim to generate a brain tumor biochip to examine how the heterogeneities within the tumor microenvironment impact glioma growth, and the biophysical conditions that limit therapeutic efficacy. This tool has the potential to combine clinical data obtained from diagnosis of patients, prognosticate the cell dynamics in tumor progression and lead, as a result, to the design of personalized therapy.

5.39 Self-Organized Nanolayering Induced by Sliding Wear in Cu-Ag two phase alloy

Fuzeng Ren (fzren@illinois.edu), Salman Arshad, Pascal Bellon, Robert S. Averback
Department of Materials Science and Engineering, UIUC

Design of bulk materials/surfaces with exceptional resistance to contact deformation and damage poses a grand challenge for their applications in harsh environment. Severe plastic deformation (SPD) of the contacting surfaces induced by sliding friction often causes localized material failure and wear. However, in some cases, sustained deformation by driving materials far from equilibrium can trigger the formation of self-organized nanostructures with improved wear resistance. Here, we report a novel self-adapting behavior by spontaneous formation of chemically nanolayered structures in Cu-Ag two-phase alloy during sliding wear. With controllable initial

Ag precipitate sizes, the nanolayered structures are stable up to the sliding surface, leading to a reduction of wear rate and inverse trend to Archard's Law. Chemically nanolayered structures are also observed in the same alloys deformed by high pressure torsion. These results offer unprecedented opportunities and deep insight into designing wear-resistant bulk metallic nanocomposites for wear applications in extreme environments.

5.40 Integrated Meta-Omics: the New Frontier for Environmental Engineering

Huijie Lu (hl2409@illinoise.edu), Wen-Tso Liu
Civil and Environmental Engineering, UIUC

Treating waste is no longer the sole purpose of implementing environmental biotechnologies. Environmental scientists and engineers are striving for sustainability by reducing greenhouse gas emissions, reusing high-quality water, and recovering energy and resources from waste. To achieve these goals, continuous knowledge improvement in community-level metabolic potentials, gene regulation, species interactions and their relationships with the surrounding environment is essential. I strongly believe that unlocking these complexities is the key in revolutionizing environmental biotechnology in the new era. Molecular and systems biology have showed great potentials in unraveling the full genetic blueprint, functional profiling and dynamics of microbial communities in soil, ocean and sediments. However, their applications in environmental engineering biosystems have been very limited so far. My research focuses on applying high-throughput, omics-based systems biology and molecular biology to resolve challenges in sustainable water and wastewater treatment. The overarching goal is to build more complete structural and functional networks for water and wastewater bioreactors, better model the succession of microbial communities, and potentially re-engineer biological treatment processes towards energy and resource sustainability.

5.41 Allelopathic effects of horseradish leaf tissue extract on lettuce seeds

Kang Mo Ku (ku8@illinois.edu), Mosbah M. Kushad, John A. Juvik
Department of Crop Science, UIUC

Previous study revealed that allyl isothiocyanate which is the hydrolysis product of the glucosinolate, sinigrin, prevalent in horseradish root and leaf tissues has allelopathic effects on the germination of weed and crop seeds. The sinigrin in horseradish leaf tissue could be utilized as weed control agents. This study measured sinigrin, its hydrolysis product, and germination inhibitory activity on lettuce seeds by using aqueous solution of horseradish leaves from different lines. There was significant negative correlation between sinigrin concentrations and root growth of lettuce seeds of extracts from different horseradish lines ($r^2=0.82$, $p=0.005$). In order to investigate the mechanism of root elongation inhibition, RNA from germinating lettuce seed was collected at 0, 4, 8, 12, 16, and 20 hours after exposure to aqueous horseradish leaf extracts (AHLE) as well as controls. RNA transcript abundance of lettuce gibberellin 3 oxidase 2 and ACC synthase at 4 and 12 hour were significantly reduced in the treatment group compared to controls. In addition, antioxidant enzyme related genes, Cu/Zn superoxide dismutase and glutathione peroxidase were significantly increased in the AHLE treatment group at 16 hour exposures. This indicates that AHLE inhibits root elongation by retarding gibberellin and ethylene gene expression.

5.42 Contamination particle source in high vacuum deposition systems

Ivan Shchelkanov (shchelkanov.ivan@gmail.com), A.M. Lietz, D.N. Ruzic
Department of Nuclear Plasma and Radiological Engineering, Center for Plasma-Material Interactions

Extreme UltraViolet Lithography (EUVL) requires reflective mask blanks, manufactured by ion beam sputtering a multilayer stack of thin films, primarily Mo and Si, onto a mask substrate. At least 40 bilayers of Mo and Si are necessary to produce on a surface. When contaminant particles deposit between these layers, the EUV light is absorbed or scatters irregularly, rendering the mask blank unusable. One possible source of such particles is bombardment of shields in the deposition chamber by energetic particles scattered from the ion beam and target and "overspill" of the tails of the ion beam off the edge of the target under oblique target angle of incidence. Shields are used to cover targets that are not in use and prevent deposition or sputtering nearby surfaces and equipment. These shields must be able to accept many successive layers of deposition without flaking and forming particles of deposited material. Shields of various materials and surface finishes were compared to determine the lowest level of particle formation. Particle sizes and shapes were quantified with high resolution SEM imaging of the shields before and after treatment to check for qualitative features, such as plateau formation, that may indicate the mechanism of particle formation.

5.43 Haloacetamide and haloacetonitrile formation from the reaction of Monochloramine and Aldehydes in drinking waters

Susana Y. Kimura (skimura2@illinois.edu), Yukako Komaki, Michael J. Plewa, Benito J. Marinas
Civil and Environmental Engineering, UIUC

Chloramination is increasingly being used because it can provide a stable residual in drinking water distribution systems and it can produce lower levels of regulated disinfection by-products (DBPs) that are predominantly formed by free chlorine. However, chloramination can promote the formation of unregulated nitrogen-containing disinfection by-products (N-DBPs) such as haloacetonitriles and haloacetamides that have been found to be more cyto- and genotoxic than regulated DBPs. Previous studies have shown that monochloramine react with aldehydes, common ozone and chlorine DBPs, to form carbinolamines that can then slowly dehydrate to imines which quickly decompose to nitriles. Additionally, carbinolamines can be oxidized to amides under mild conditions. In this research, the formation of chloroacetonitrile and N,2-dichloroacetamide from the reaction of monochloramine and chloroacetaldehyde is investigated. Chloroacetaldehyde and monochloramine react and reach equilibrium with carbinolamine 2-chloro-1-(chloroamino)ethanol. This carbinolamine decomposes through two concurrent

pathways 1) a slow dehydration to 1-chloro-2-(chloroimino)ethane, which in turn decomposes quickly to chloroacetonitrile, and 2) oxidation by monochloramine to form N,2-dichloroacetamide. These reactions are acid/base catalyzed, and therefore, the rates of formation of chloroacetonitrile and N,2-dichloroacetamide are highly influenced by water quality conditions. A kinetic model is provided to predict N-DBP formation and aid in developing strategies for N-DBP control.

5.44 The role of CO2 and ionic liquid complex on the electroreduction of carbon dioxide at lower potentials

Natalia Garcia Rey (ngarciar@illlinois.edu), Bruno N. Giuliano, Richard L. Masel, Dana Dlott
Chemistry, University of Illinois

Artificial photosynthesis is one of the answers to help to address global warming and to sustainable energy products. To the date, a big deal of progress has been done in the reduction of carbon dioxide to obtain a variety of organic compounds. This reaction nevertheless needs to meet two criteria: high energy efficiency and high reaction rates to become feasible. Masel's group recently reported a very promising advance in the field, reducing carbon dioxide at 0.3 V instead of 1V (Rosen et al. Science 334 (2011) 643). Ag nanoparticles and Pt electrodes immersed in ionic liquid and water as electrolyte media composed this electrochemical cell, producing carbon monoxide and hydrogen. Ionic liquids are salts liquid at room temperature, environmentally friendly and with a range of properties due to their tunability. In this work we have studied the complex formation of the carbon dioxide and EMIM-BF_4 in the vicinity of the electrode. A state of art vibrational spectroscopy is carried out following up the steps of the reaction when a negative potential is applied. These new insights in the electrochemical reduction of carbon dioxide on the electrodes help to improve the cell to become economically viable.

NOTES

Please leave this page in the collection box at the Registration table prior to the reception

Vote for the Best Talk

Please check **three** talks you enjoyed most

Session 1

- ○ 10:15 – 10:30 Juan Perilla (1.1)
  Molecular mechanisms of HIV infection
- ○ 10:30 – 10:45 Sarah Erickson-Bhatt (1.2)
  In vivo intra-operative breast tumor margin detection using a portable OCT system with a handheld surgical imaging probe
- ○ 10:45 – 11:00 Sheng Xu (1.3)
  Hard-soft integrated multifunctional devices for mobile healthcare systems
- ○ 11:00 – 11:15 Venkatraman Srinivasan (1.4)
  Fewer not more leaves - Key to obtaining the needed jump in crop yield potential
- ○ 11:15 – 11:30 Craig Yendrek (1.5)
  Exploiting inter-specific variation to improve abiotic stress tolerance in crops

Session 2

- ○ 11:45 – 12:00 Mostafa Elag (2.1)
  Data network
- ○ 12:00 – 12:15 Catello Di Martino (2.2)
  Lessons learned from the failure analysis of Blue Waters
- ○ 12:15 – 12:30 Robin Berthier (2.3)
  Challenges and solutions for a resilient power grid
- ○ 12:30 – 12:45 Yukako Komaki (2.4)
  Analyses of cell cycle alteration induced by haloacetonitriles: Toxicity of drinking water disinfection by-products
- ○ 12:45 – 1:00 Aaron Finck (2.5)
  Vortices and gate-tunable bound states in a topological insulator coupled to superconducting leads

Session 3

- ○ 3:00 – 3:15 Christopher Mayne (3.1)
  Force field toolkit: Rapid parameterization of small molecules for use in biomolecular simulations
- ○ 3:15 – 3:30 Oya Okman (3.2)
  Self-healing in Li-ion battery electrodes
- ○ 3:30 – 3:45 Chi Hwan Lee (3.3)
  Transfer printing method for flexible, cheap and light-weight thin-film electronics
- ○ 3:45 – 4:00 Rui Zhang (3.4)
  Accelerated self-replication under non-equilibrium, periodic energy delivery

Session 4

- ○ 4:15 – 4:30 Emmanuel Nuesiri (4.1)
  All adaptation is local: Local government capacity and climate change
- ○ 4:30 – 4:45 Rodica Damian (4.2)
  Psychopathology, adversity, and creativity: Diversifying experiences in the development of eminent African-Americans
- ○ 4:45 – 5:00 Alex Konkel (4.3)
  They can take a hint: Preserved integration of outside information with memory in older adults
- ○ 5:00 – 5:15 Audrey Michal (4.4)
  The role of attentional shifts in graph comprehension

INTENTIONALLY BLANK

Please leave this page in the collection box at the Registration table prior to the reception

Vote for the Best Poster

Please check **three** posters you enjoyed most

- ○ 5.1 **Yanjing Li** *Transition of Localization Behavior in MoS2 Nanoribbon*
- ○ 5.2 **Keith Cassidy** *The Bacterial Brain: Looking into a Chemoreceptor Array*
- ○ 5.3 **Min Kyung Lee** *Colloidal Particle Assembly in Microchanneled, Bioactive Hydrogel for Vascular and Neural Patterning*
- ○ 5.4 **Canan Dagdeviren** *Conformal Piezoelectric Energy Harvesting and Storage From Motions of the Heart, Lung and Diaphragm*
- ○ 5.5 **Boon Chong Goh** *Molecular Modeling of the Immature Retroviral Lattice*
- ○ 5.6 **Jennifer Maier** *The Opossum: A New Model for Intervertebral Disc Development?*
- ○ 5.7 **Renee Sadowski** *Oral administration of bisphenol A during early development alters adult neuron and glia number in the prefrontal cortex of male, but not female, rats*
- ○ 5.8 **Wan-Ting Chen** *Hydrothermal Liquefaction of Mixed-culture Algal Biomass from Wastewater Treatment System into Bio-crude Oil*
- ○ 5.9 **Kishor Kumar Kalathiparambil** *Erosion effects on tungsten plasma facing components*
- ○ 5.10 **Hyang Yeon Lee** *Potent and Selective Synergistic Effect of NHI-Glc-2 and DNQ Combination in Cancer Treatment*
- ○ 5.11 **Mei-Hsiu Lai** *Tailoring Polymersome Bilayer Permeability for Improved Tumor Detection and Imaging*
- ○ 5.12 **Priya Raman** *Optimized Magnetic Field Configuration for High Power Impulse Magnetron Sputtering*
- ○ 5.13 **Sumin Kim** *Controlled and Safer Therapeutic Delivery of Venom Peptides using Well-defined Polymeric Nanoparticles for Cancer Inhibition*
- ○ 5.14 **Santosh Misra** *Nanocelles for Improved Inhibition of Breast Cancer Stem Cells via STAT-3 Cascade Pathway*
- ○ 5.15 **Aram Yoon** *Understanding oxidation in atomic scale*
- ○ 5.16 **Dawn Eriksen** *Pathway Engineering through Simultaneous Directed Evolution of Multiple Biosynthetic Pathway Proteins*
- ○ 5.17 **Bala Mutyala** *Bullying in Illinois Public Schools*
- ○ 5.18 **Syed Abbas Bukhari** *Socially Responsive Gene Families Are Conserved For Male-Male And Male-Female Social Interactions In Fruit Fly And Stickleback Fish*
- ○ 5.19 **Sung Jun Lim** *Brightness-equalized quantum dots for quantitative biological imaging*
- ○ 5.20 **Anabelle Couleau** *Price Volatility Interdependence in the European Biodiesel Industry over and across Markets*
- ○ 5.21 **Jaime Thissen** *Community-Based Approaches to Addressing Agroecological Integrated Systems in the Brazilian Amazon Rainforest*
- ○ 5.22 **Aldis Sipolins** *Anodal tDCS during videogame training enhances transfer to the Stroop Effect*
- ○ 5.23 **Amanda Marciel** *Fluidic-directed assembly of aligned oligopeptides with pi-conjugated cores*
- ○ 5.24 **Danielle Mai** *Flexible Branched Polymers for Single Molecule Rheology*
- ○ 5.25 **Daniel Reilly** *Engineering Fluorescent Dendrimer Nanoprobes for Increased Photostability*
- ○ 5.26 **Laura Mozdzen** *Spatially-graded collagen biomaterials to regenerate the tendon bone junction*
- ○ 5.27 **Xinxin Feng** *Structures of bacterial diterpene and isoprenoid synthases: Targeting virulence and biofilm formation*

- 5.28 **Yugang Bai** *Synthesis and application of single-chain polymer nanoparticles*
- 5.29 **Sayan Bhattacharyya** *Investigating writers' attitudes by mining a large corpus of books*
- 5.30 **Youhua Tan** *Matrix softness regulates plasticity of tumor-repopulating cells via H3K9 demethylation and Sox2 expression*
- 5.31 **Santosh Misra** *Regressing Metastatic and Drug Resistant Breast Cancer with Trigger-able Pro-nifuroxasome Nanoparticle by Inhibiting Transcription Factor STAT3*
- 5.32 **Jun Wu** *α-Catenin cytomechanics: role in cadherin-dependent adhesion and mechanotransduction*
- 5.33 **Yu-Hsiang (John) Huang** *IT Portfolio Efficient Frontier and Decision Making*
- 5.34 **Brian Metzger** *Not all probes are created equal: Suppressed-eye probes draw attention to the suppressed eye*
- 5.35 **Han Xiao** *Exploiting Issatchenkia orientalis SD108 for Succinic Acid Production*
- 5.36 **Masoud Safdari** *An Isogeometric Interface-enriched Generalized Finite Element Method for Problems with Complex Discontinuous Gradient Field*
- 5.37 **Jialan Zhang** *Free energy of compositionally graded ferroelectric films*
- 5.38 **Sara Pedron** *3D hydrogel platforms to study glioblastoma malignancy*
- 5.39 **Fuzeng Ren** *Self-Organized Nanolayering Induced by Sliding Wear in Cu-Ag two phase alloy*
- 5.40 **Huijie Lu** *Integrated Meta-Omics: the New Frontier for Environmental Engineering*
- 5.41 **Kang Mo Ku** *Allelopathic effects of horseradish leaf tissue extract on lettuce seeds*
- 5.42 **Ivan Shchelkanov** *Contamination particle source in high vacuum deposition systems*
- 5.43 **Susana Y. Kimura** *Haloacetamide and haloacetonitrile formation from the reaction of Monochloramine and Aldehydes in drinking waters*
- 5.44 **Natalia Garcia Rey** *The role of CO2 and ionic liquid complex on the electroreduction of carbon dioxide at lower potentials*