

2012 IGERT Annual Meeting

Technical Session IV Abstracts

Nanoscience and Materials Science

Craig Arnold, Princeton University

Nanotechnology and Energy Research in a Macro World

Johanna Bernstein¹, and Manish Chhowalla², Craig B. Arnold³

¹ Institute for Advanced Materials, Devices and Nanotechnology, Rutgers, The State University of New Jersey, Piscataway, NJ 08854. ² Department of Materials Science and Engineering, Rutgers, The State University of New Jersey, Piscataway, NJ 08854 ³ Department of Mechanical and Aerospace Engineering, Princeton University, Princeton, NJ 08504.

Economic, environmental, strategic and societal issues have placed energy-related topics at the forefront of research in a broad and diverse range of areas. For nanotechnology, particular, these issues encompass everything from fundamental technological advances in electronics and photonics, to advances in the engineering of photovoltaic materials and devices. The Rutgers-Princeton IGERT explores the connections between nanotechnology and clean energy with particular emphasis on research that cuts across traditional disciplines and incorporates various areas of expertise. In this presentation, we will highlight selected research activities in our IGERT that exemplify our program. For instance, research related to improved efficiency in nanoparticle enhanced photovoltaic devices, the effects of nanoscale materials in electrochemical devices, and scaling technologies for nanomaterials in power electronics will be discussed. In addition to the particular research endeavors, this presentation will demonstrate how the trainees are able to take advantage of a unique combination of resources from multiple disciplines and geographically dispersed universities and institutes as part of a unique community of scholars.

Mary Berry, University of South Dakota

There has been a recent explosion of interest in upconverters (UC) for device and sensing applications, owing to the introduction of efficient, solvent-dispersible nanocrystalline UC materials (NaYF₄) activated by trivalent lanthanide ions (Ln³⁺). The use of upconverters in a nanocrystalline form dramatically increases their processability, in terms of incorporation into composite materials, and provides high spatial resolution and biocompatibility for sensing applications. However, it is difficult to directly measure the quantum efficiency of these materials, and the effect of materials parameters on efficiency (such as particle size, capping ligand, composite matrix) is poorly understood. A rate-equations model has been constructed which describes the mechanism of NIR-to-visible upconversion in NaYF₄:Er, Yb in terms of the microscopic rate constants relevant to the upconversion mechanism. This model can be used to determine NIR-to-visible quantum efficiency from accessible spectroscopic data, and can isolate the effects of nanoparticle size, doping concentrations, etc. on the individual mechanistic steps. The use of the model in characterizing the potential for enhancing upconversion using plasmonic surfaces will also be discussed.

Suely Black, Norfolk State University

The IGERT-MNM research combines interrelated areas of photonic, magnetic and nanostructured materials and devices seeking to achieve varied scientific and engineering advances afforded by the interdisciplinary collaboration. Brief summaries of recent results of three research projects are outlined below:

1. Hyperbolic metamaterials are an important class of metamaterials, in which values of dielectric permittivities in orthogonal directions have opposite signs. These materials enable a variety of applications ranging from a hyperlens to a perfect absorber. We have demonstrated that absorption of thin dye-doped polymeric films can be tuned and enhanced (nearly threefold) by lamellar metal-dielectric hyperbolic metamaterial substrates, compared with traditional dielectric substrates. We have also demonstrated a drastic reduction of reflectance from hyperbolic metamaterials, enabled by their curvilinear shapes as well as scatterers placed on their surface.

2. Magnetic nanoparticles (MNP) are important for many applications in industry, science, and medicine. Our fundamental studies demonstrate the applicability of quantization approach to magnetization dynamics of MNPs. Ultra-small MNP were shown to be suitable for design of tunable metamaterials, in which propagation of electromagnetic waves can be controlled with external magnetic fields. Most efficient size of MNPs for magnetic resonance T1-related imaging applications in viscous biological media has also been determined.

3. The combination of magnetic and dielectric materials forming multiferroic behavior offers a new class of materials for magnetic, sensor as well as metamaterials through tuning of properties. We have fabricated and characterized a multilayer structure consisting of magnetic and ferroelectric/piezoelectric layer in which both magnetism and electric polarization can be manipulated.

Guann-pyng Li, University of California, Irvine

Concurrent revolutions in biology, medicine, physical sciences and engineering at the micro/nano scale, accompanied by advances in instrumentation, are bringing these separate disciplines into convergence. This exciting trend has potential to bring important changes to life science and technology. LifeChips is the study of nature's 3 billion years of evolution and development of micro/nano-scale technologies, systems and devices that combines methods developed by life scientists and technologists to help solve fundamental problems. UCI is spearheading development in LifeChips by creating nanotechnology and medical device research programs, developing design methodologies, defining new applications, promoting commercialization, and pursuing novel manufacturing techniques. LifeChips research projects at UCI provides examples of potential new discoveries, including implantable microdevices, minimally invasive devices, cell analysis chips, and biosensors. In addition to utilizing micro/nano chip technologies, each project and device has unique requirements for design, manufacture and deployment. These requirements drive the need for advances in micro/nano fabrication and system-integration at manufacturing level, building the foundations for a new LifeChips industry.

Xiaoquin (Elaine) Li, University of Texas at Austin

Lego approach to plasmonics

Metallic nanoparticles (NPs) exhibit rich and unique optical properties due to surface plasmon modes. When NPs are placed in close proximity of each other, the possibility of shaping and controlling near field and far field optical properties expands enormously. Near-field coupling between plasmonic NPs is sensitive to nanometer geometric changes of constituent components. This strong dependence on geometry provides exciting opportunities in confining and manipulating optical field on the nanoscale, though at the same time presents serious challenges in the fabrication and characterization of the plasmonic nanostructures. We use the method of nanomanipulation with an atomic force microscope to assemble well-defined plasmonic nanostructures and investigate the optical properties of such individual structures. I will discuss two particular examples: 1) the simplest active plasmonic structure consisting of a gold sphere and a semiconductor quantum dot. and 2) a plasmonic protractor consisting of a gold sphere and a rod.

Taher Saif, University of Illinois at Urbana-Champaign

Elasticity of microenvironment and cancer metastasis

Cancer deaths are mostly caused by metastasis of malignant cells, not by the tumor itself. During metastasis, cancer cells turn off adhesion ability, de-adhere from their neighbors or the extracellular matrix (ECM), enter the lymphatic system or the blood stream as suspensions, invade new host tissues, regain adhesive activity and form new colonies. Thus, cell adhesion plays a central role in metastasis. Here we show, for the first time, that mechanical stiffness of cancer cells' microenvironment may determine the fate of cell adhesion and subsequent metastasis. We culture human colon cancer cells (HCT-8) on PA gel substrates with different stiffnesses, very soft (1KPa gel) to stiff (40KPa gel) to very hard (3GPa standard plastic Petri dish). We find, on intermediate stiffness (20-40KPa) substrates, the cells first form tissue or tumor like clusters with strong cell-cell adhesion mediated by cell adhesion molecule E-Cadherin. On the 7th day of culture, the cells begin to down-regulate cell-cell adhesion. They detach from the tumors, significantly lower E-Cadherin content, become migratory or invasive, proliferate rapidly, and become lubricated (non-adhesive), i.e., they show many of the critical hallmarks of in vivo metastasis. Essentially the cells undergo a transition of state, from epithelial to mesenchymal, common during the onset of cancer metastasis. On very soft or very hard substrates, cells do not show this transition. Actin and nuclear staining show high intracellular forces on hard substrate and intermediate forces on 20-40KPa gel substrates. Reduction of forces by inactivating motor protein, myosin II, inhibits the transition. Taken together, it appears that the magnitude of intracellular forces is determined by the elasticity of the microenvironment, and the intracellular forces determine the fate of cell-cell adhesion over time and hence the onset of metastasis.

Srinivas Sridhar, Northeastern University*Theranostic Nanoplatfoms for Image-Guided Drug Delivery and Radiation Oncology*

Biocompatible nanomaterials are key components of novel approaches to addressing the major problems of disease diagnosis and therapy. We have developed several nanoplatfoms that offer potential for significant improvements in multi-modal imaging and targeted delivery of therapeutics. Magnetic liposomal nanoplatfoms for theranostics combine multiple functionalities including imaging, magnetic targeting to the disease site, delivery of the drug payload through sustained as well as triggered drug release. We have demonstrated in vivo multimodal imaging using MRI, SPECT and FMT using these nanoplatfoms.

We have developed a new approach to local chemoradiation therapy (CRT), termed Biological In-Situ Image Guided Radiation Therapy, that involves the coating of spacers routinely used during radiation therapy with nanoparticles that release radiosensitizing drugs (e.g. docetaxel DTX for Prostate Cancer), that is synchronized with the radiation therapy schedule, with almost no systemic toxicity. This new nanoparticle approach is an exciting new combinatorial therapy for cancer as well as other diseases where image-guided radiation therapy is currently a preferred choice of treatment.

Haskell Taub, University of Missouri, Columbia*Study of water diffusion on single-supported bilayer lipid membranes by quasielastic neutron scattering*

Our interdisciplinary team of physicists, chemists, biochemists, and instrument scientists is using neutron scattering and molecular dynamics simulations to elucidate the motion of water molecules associated with single bilayer lipid membranes supported on a silicon substrate. This system serves as a model of biological membranes that surround all living cells. Knowledge of the water structure and its dynamics is important for understanding the membrane function. We have performed high-energy-resolution quasielastic neutron scattering experiments at NIST and at Oak Ridge National Laboratory. By varying sample temperature, level of hydration, and deuteration, we have identified three different types of diffusive motion in membrane-associated water: bulk-like, confined, and bound [1]. The motion of bulk-like and confined water molecules is fast compared to those bound to the lipid head groups (7-10 H₂O molecules per lipid), which move on the same nanosecond time scale as H atoms within the lipid molecules.

1. M. Bai, A. Miskowiec, F. Y. Hansen, H. Taub, T. Jenkins, M. Tyagi, S. O. Diallo, E. Mamontov, K. W. Herwig, S.-K. Wang, *Europhys. Lett.*, in press.

Bioinformatics and Bioengineering

Kimberly Anderson, University of Kentucky (unable to attend)

NSF IGERT and REU Programs in Engineered Bioactive Interfaces and Devices: An Integrative Approach

The University of Kentucky has directed IGERT and REU Programs on Engineered Bioactive Interfaces and Devices. This multidisciplinary area focuses on the novel design of architectures that interact with biological systems and promote a desired response. These advanced architectures have numerous applications ranging from tissue engineering to sensing systems to drug delivery. Successful development of these systems depends on expertise not only in developing novel synthetic architectures through nanotechnology, self-assembly and hybrid systems but also on the interactions of these interfaces with biological systems such as cells and proteins. Both research developments and educational aspects of the programs will be presented.

Gary Benson, Boston University

A Computational Pipeline for Detecting Tandem Repeat Variants in Next-Generation Sequencing Data

Analysis of the 454 Watson Genome...The tandem repeats (TRs) are a ubiquitous class of genomic features, each one consisting of a pattern of nucleotides which is repeated, either exactly or approximately, two or more times in tandem, as adjacent copies. Across the class, the actual pattern, pattern size, and number of copies is highly variable. TRs undergo copy number expansion or contraction mutations, in which one or more copies is gained or lost. Although these tandem repeat polymorphisms (TRPs) have been observed for a number of well study loci, little is known about genome wide occurrence of TRPs, that is, which TRs are TRPs, what alleles (copy numbers) exist, and what the allele frequencies are in the population. Since TRs often occur in gene promoters and other chromosome functional regions, their variability may have unattributed regulatory effects. We report on our development and application of a computational pipeline to analyze next-generation sequencing data in order to discover TRPs, using the James D. Watson genome as a test case. Our pipeline predicts 719 VNTRs in the Watson genome, using low coverage data.

Bir Bhanu, University of California, Riverside

This collaborative project brings together an interdisciplinary team of investigators from Engineering, Computer Science and Life Sciences in an integrated effort to train the next generation of scientists and engineers to enable the study of 5-D (3-D space, time and wavelength) biological processes captured live by video in real-life experiments. The advances of live cell video imaging and high-throughput technologies for functional and chemical genomics provide unprecedented opportunities to understand how biological processes work in subcellular and multicellular systems. However, traditional curricular structure does not provide the biological scientist with the foundation to develop video computing techniques, nor does it provide the engineer with an understanding of the significance of critical current biological issues which 5-D analysis can help illuminate. This IGERT trains students at the forefront of science and technology in biological video computing which provides foundational advances and a deeper understanding of continuous and dynamic life processes involved with cells, organisms, and disease.

Thomas Cech, University of Colorado at Boulder

Non-coding RNAs Genome-Wide: The Interface of Genomics and Computation

Tom Cech^{1,2}, Robin Dowell^{1,3,4}, Manuel Lladser⁵, Rob Knight^{1,2,4}, Andrea Stith¹ and Jana Watson-Capps¹
¹Univ. of Colorado BioFrontiers Institute, ²Dept. of Chemistry & Biochemistry, ³Dept. of Molecular, Cellular & Developmental Biology, ⁴Dept. of Computer Science, ⁵Dept. of Applied Math, , Univ. of Colorado, Boulder, CO 80309

The roles of ribonucleic acid molecules as messengers (mRNA) and as active participants in protein synthesis (rRNA and tRNA) are well known. More recently, it has been discovered that RNA can do much more: some RNA molecules act as biocatalysts, while tens of thousands of long non-coding RNAs transcribed from the human genome have functions in transcriptional regulation that are only beginning to be unraveled. The PI and several of the co-PIs and students in the University of Colorado IQ Biology PhD certificate program are working in this area. The Cech lab has found a new mechanism by which the FUS protein regulates human transcription by binding to RNA polymerase II in a non-coding RNA-dependent manner. The Dowell lab has found that non-coding transcription allows yeast to switch from smooth colony formation to an invasive, filamentous form. The Knight lab, on the other hand, uses a non-coding RNA (16S rRNA) to analyze the complexity of the microbiome. The common denominator of these projects is that molecular biologists must work in close conjunction with computer scientists and applied mathematicians to glean new information from enormous DNA sequence datasets. One of the goals of IQ Biology is to train a cadre of students who understand the biological problems and can develop computational tools to make an impact on research involving non-coding RNAs.

Robert Full, University of California Berkeley

Leaping Lizards, Bio-inspired Robots and Dinosaurs

The study originated in our IGERT discovery-based teaching laboratory housed in Berkeley's Center for interdisciplinary Bio-inspiration in Education and Research (CiBER; <http://ciber.berkeley.edu>). Leaping African, Red-headed lizards control tumbling by careful swings of their tails. Testing a 40 year-old hypothesis first proposed for dinosaurs like those of Jurassic Park fame, lizards ran down a track, and vaulted off an obstacle, as in the Olympics. Instead of landing on the ground, they leapt to a vertical surface with a safe shelter on top. When the friction on the obstacle was reduced, lizards slipped, potentially causing their body to spin out of control. Using high-speed videography and motion capture, we noticed that while airborne, the rotation of their body appeared to be solely counteracted by the swing of their tail up or down, keeping them stable. To see if the tail was actively stabilizing the lizard's body in mid-air, we used a control theoretic approach from engineering. To quantify our observations, we built both mathematical and physical models. The lizard-sized, physical model took the form of an active tailed robot car we named Tailbot. With no feedback from sensors about body position, the robot took a nose-dive when driven off a ramp that mimicked the lizard's take-off. However, when body attitude was sensed and fed back to the tail motor, Tailbot's body was stabilized by redirecting the angular momentum of the body into the swing of the tail, just like the leaping lizards. Tailbot isn't only a model for biology, but it also pushes the boundaries of control in robotics in an area we term, Inertial Assisted Robotics.

Bin He, University of Minnesota*Fly High with Your Thoughts: A Systems Neuroengineering Approach*

Systems Neuroengineering (sNE) is an emerging interdisciplinary field that uses engineering principles and techniques to understand, repair, restore, enhance and otherwise exploit the properties of nervous systems. We have explored a novel noninvasive neural interfacing system to decode humans' intentions from EEG signals based on principles of sNE. We have demonstrated the capability to control the flight of an AR.Drone by the "thoughts" of human subjects. Experimental studies have been conducted to delineate mechanism of brain activation during motor imagery tasks. Novel techniques are developed to reliably decode the extremely weak brain signals associated with the "thoughts" during motor imagery. In this novel brain-machine interface, action is planned in the human's brain, signals decoded and transformed into control signals that are transmitted via a wireless network to control continuously the flight of an AR.Drone. This work demonstrates the potential for enhancing functions of healthy subjects and for restoring capabilities of interacting and controlling the environment for disabled patients.

Todd McDevitt, Georgia Institute of Technology

Stem cell biomanufacturing is the conduit for fundamental scientific discoveries about stem cell biology to be translated into biomedical diagnostics and therapies. Robust new approaches to control the expansion and differentiation of stem cells in a scalable manner are required for cell production purposes. In addition, non-destructive means of assaying cell fate are needed to introduce feedback-control processes and ensure the safety and efficacy of stem cell-derived products. These objectives are being met by the research currently being carried out by Stem Cell Biomanufacturing IGERT trainees at Georgia Tech who are preparing to become the scientific leaders of this rapidly emerging field that exists at the crossroads of stem cell biology, bioengineering and bioprocessing. Specific research efforts include the development of biomaterials approaches for the culture and delivery of stem cells, computational modeling of stem cell fate decisions, label-free non-destructive cell sorting technologies and "real-time" gene expression analysis. Overall, these projects represent the next generation of technologies to be integrated into the biomanufacturing pipeline for the production and ultimately translation of stem cells for biomedical applications.

Karen McDonald, UC Davis

Plants are a vast renewable source of important natural products, and the development of genetic engineering approaches has opened up a myriad of new possibilities for extending the biosynthetic capabilities of plants by enabling the production of heterologous proteins and new metabolic pathways in whole plants, plant tissues and in-vitro systems such as plant cell cultures in bioreactors. Although plant biotechnology has been deployed commercially for decades for improved agronomic traits of crops, the combination of new expression technologies and synthetic biology building blocks for plants, rapid and inexpensive DNA synthesis, and novel bioprocessing strategies are enabling plants to be used as molecular foundries to solve some of our most important societal problems in health and energy in an environmentally-friendly way. For example, new production platforms based on transient expression in nontransgenic plants within contained manufacturing facilities are showing enormous promise for rapid, scalable production of vaccines, without the need to deploy transgenic plants and eliminating many of the environmental concerns. A soil bacterium, *Agrobacterium tumefaciens*, that has an inherent capability of interkingdom DNA transfer, is used to introduce the genetic instructions into plant cells. Plant cells within the plant tissues then provide the biosynthetic machinery for transcription, translation, post-translational modifications, folding and intracellular targeting/secretion of the product. Thus the approach combines the advantages of rapid, easy and inexpensive growth of bacteria in fermentation systems with the biosynthetic capabilities of higher eukaryotic cells which have been grown using

minimal energy and resource inputs (using sunlight and natural resources). Advances in this field require interdisciplinary teams combining expertise in plant science, molecular biology, bioprocess engineering, microbiology, and plant pathology, as well as an understanding of the regulatory, economic and IP constraints. This new technology will be described along with results from CREATE-IGERT trainees' research projects focusing on biofuel and biodefense applications.

Climate, the Environment, and Ecology

David Andow, University of Minnesota

GM-crop unintended ecological effects on organisms

Genetically-modified (GM) crops have been grown in the US for 16 years. Accumulated experience with GM-Bt crops has highlighted the need to improve environmental risk assessment (ERA) so that concerns to society can be assessed, and to predict secondary pest outbreaks. Three cases illustrate these points. 1. Concerns about monarch butterfly and GM-Bt maize became widely known about 12 years ago. Monarch butterfly is not endangered or critical for any ecosystem service, but was valued because it is a species of cultural concern in the US, a new kind of ecological risk that was not considered. 2. ERA typically evaluates effects via a tiered assessment procedure, assuming that if no effect is detected in early trials, there will be no effects in later trials. A meta-analysis for several GM crops revealed that unacknowledged effects occurred in early laboratory trials, suggesting that the standard tiered procedure needs to be improved. 3. GM-Bt crops can cause secondary pest outbreaks, such as plant bugs on Bt cotton in China, and stink bugs on Bt cotton in the US. Because they are difficult to predict in advance, a strong agricultural extension service is essential to maintain the benefits of Bt crops. This social cost must be considered a part of the cost of using GM crops.

Lee Fitzgerald, Texas A&M University

Solutions to the biodiversity crisis will ultimately come from biological and social scientists working in tandem, yet disconnects among disciplines, conservation institutions, and practical implementation hinder effective conservation. The vision of Applied Biodiversity Science (ABS) is to achieve integration between biodiversity research and conservation practices. Three pillars support ABS: 1) integrated social and biological research; 2) cross-disciplinary collaboration with local institutions and actors; and 3) application of conservation theory to practice. Our ABS program is focused on two cross-cutting themes: Ecological Functions and Biodiversity; and Communities and Governance. We designed a research integration matrix that matches causes of biodiversity loss against research approaches, and explain how this tool can be used to define integrative questions and build interdisciplinary research teams. Case studies from the Amazon and Gran Chaco illustrate how we are implementing the ABS model. Our intention is that ABS approaches will produce conservation scientists who communicate effectively across disciplines, and make their research relevant to programs. The ABS approach elucidates how ecosystem function, biodiversity, and governance systems are interconnected.

Elise Granek, Portland State University

Growing urban areas depend on ecosystem services: Many studies have documented the growing fragility of a majority of the globe's ecosystems. Policymakers and resource managers often frame such ecosystem challenges as primarily about protecting natural systems in rural areas. However, that conception misses a key part of the story: the rapid growth of urbanizing areas. Home to more than 50 percent of the world's human population for the first time in modern history, urbanizing regions concentrate pressure on ecosystem services, which are necessary to sustain healthy urban living conditions and vibrant commerce. This dramatic urbanization presents both challenges and opportunities for novel ecosystem services management. A transdisciplinary framework is needed to discover innovative solutions to these wicked problems because they involve complex relationships between natural and human systems, link natural, rural and urbanizing regions and transcend any single discipline. The framework should integrate natural and social sciences with stakeholders' intimate knowledge of ecosystem services and urban systems. Here we describe such a framework for training scientists and managers and present four novel cases that illustrate ecosystem management solutions for urbanizing areas. ESUR IGERT students are testing this framework in collaboration with community partners working in government agencies, non-profit organizations and business firms.

Rick Grosberg, University of California, Davis

Rangeland provides essential habitat for native plants and animals, conserves important ecosystem functions, and is threatened by relentless pressure from urban development and potentially climate change. The Williamson Act (WA), designed to incentivize keeping land in agriculture, reduces property taxes for owners of California farm and rangeland (over 15 million total acres). However, state budget cuts have drastically reduced WA funding. Trainees in the REACH IGERT documented the economic and environmental consequences of a scenario in which the WA program is eliminated. GIS analysis and ranch ownership records revealed that 72% of rangeland parcels enrolled in the WA contain habitat important for statewide conservation goals. In a mail survey, 71% of ranchers reported a 2009 net annual profit less than or equal to their WA property tax reduction. Under the elimination scenario, survey respondents reported intent to sell 20% of the 496,889 acres of rangeland they own, with 76% predicting that the buyers would develop the land for non-agricultural uses. This suggests substantial changes to California's landscape and impact upon its native biota in a future without the Williamson Act. These results have been shared with policymakers, ranchers, and other stakeholders.

Shafiqul Islam, Tufts University

Water Diplomacy: A Synthesis of Science, Policy and Politics for Water Management

Integration of scientific learning with the complex political reality of real-world water problem-solving remains a desirable-but-elusive goal. There is a growing consensus that solutions to most water problems need such integration. The professionals who attempt to solve water problems cannot easily translate solutions born out of scientific findings into the messy context of the real world. To bridge this divide between theory and practice - where natural, societal, and political elements cross boundaries and interact in uncertain and nonlinear way, a new approach is needed. This new approach - Water Diplomacy Framework (WDF) - is rooted in ideas of complexity theory and multi-party negotiation. We posit that water issues are better understood and managed as network of interactions and relationship among natural, societal and political processes. The WDF is based on three assumptions: (a) water is a flexible resource; (b) boundaries of water networks are open; and (c) water negotiations are designed to achieve mutual gain outcomes. Using case studies, we will show the efficacy of the WDF in managing water networks that emphasizes value-creation and adaptive problem-solving approaches.

Joane Nagel, University of Kansas

Dynamics of *Uncoupled* Natural and Human Systems

Joane Nagel, Narayani Barve, Lindsay Campbell, Anna Kern, Andres Lira-Noriega, A. Townsend Peterson, Jorge Soberon

C-CHANGE IGERT Trainees at the University of Kansas conducted research projects on conservation and sustainability: Monarch Butterflies & Local Economies in Michoacán, Mexico (2009) and Effects of Sea Level Rise on Mangrove Forests Yucatán, Mexico (2011). Interdisciplinary teams examined the fit between climate change models (of temperature and precipitation in Michoacán's Monarch preserves and sea level rise in Yucatán's mangrove restoration areas) and human conservation programs. In the case of Michoacán's monarch reserves, the lethal zones predicted by GCMs do not fit well the reserve boundaries. If the GCMs are accurate, not only the Monarchs' migration and overwintering sites will be affected, so will the local industry growing up around Monarch tourism. In the case of Yucatán's mangrove forests, federally-funded restoration efforts of local are unlikely to be effective in sustaining the mangroves from climate-change induced sea-level rise, but these efforts may continue to be funded because of policies focusing on community development. IGERT Associates used niche modeling techniques to assess the fit between several human conservation areas and the niche boundaries of species they were designed to protect.

Patricia Culligan, Columbia University

Cost Effectiveness of Green Roof Water Retention by Construction Type

Vegetated rooftops, known as green roofs, have become an increasingly popular low- impact development strategy. These systems provide a range of environmental benefits, the most documented of which is their ability to mitigate stormwater runoff. In New York City (NYC) incentive programs are offered for the construction of green roofs as part of an overall plan to reduce flooding and limit the occurrence of combined sewage overflows. The NYC incentive program, a tax break up to \$100,000, will expire on March 15, 2013; but new programs are being considered by the federal government (i.e. Clean Energy Stimulus & Investment Assurance Act) and NYC officials (i.e. PlaNYC 2030). However, for these programs to be successful it is important to: quantify the stormwater reduction of NYC green roofs and determine which construction types are most cost effective. In this study, rainfall & runoff data were collected on one full-scale extensive green roof of each construction type. Rainfall was measured using a tipping bucket rain gauge and runoff was measured using a weir chamber which was designed to fit into the downspout of existing roof drains. Results were normalized by roof drainage area and plotted to analyze trends.

Technical Session XI Abstracts

Energy and Sustainable Development

Erin Baker, University of Massachusetts, Amherst

Turning off wind turbines to reduce avian mortality

While wind power is a promising source of carbon free energy, there have been persistent questions about the safety of migrating birds in the presence of wind farms. In this paper we develop a framework that allows us to consider the costs and benefits of a very simple strategy: turning off the turbines during high-risk periods for endangered species. We develop a model that allows us to find the lowest-cost strategy for turning off turbines, given a bird-safety goal. In order to produce this model, we have combined mechanical engineering knowledge about the wind resource and the wind turbine power curve, operations research knowledge about optimization models, and the biological knowledge about of bird migration. We apply the model to a specific case study: the proposed Cape Wind project and the vulnerability of the common loon (*Gavia immer*), during one month of the migratory season. We calculate probability distributions over energy produced, price, and revenue to the wind farm, as well as over the numbers of loon mortality, and perform an uncertainty analysis. With the goal of mitigating 10 bird deaths during the month of March, we estimate that the lost revenue per bird averages \$171, using the most cost effective strategy of turning off turbines.

Renata Bura, University of Washington

Biological production of ethanol and xylitol by novel naturally occurring yeast: For economically feasible and efficient biochemical production processes, complete and fast consumption of all sugars naturally present in lignocellulosic feedstocks is required. One of the main challenges emerging from the use of lignocellulosics for the production of ethanol by the yeast *Saccharomyces cerevisiae* is efficient fermentation of D-xylose and L-arabinose, as these sugars cannot be used by natural *S. cerevisiae* strains.

In this research, a novel, naturally occurring endophytic yeast *Rhodotorula mucilaginosa* strain PTD3 was identified as being capable of rapid assimilation and catabolism of five and six carbon sugars. This yeast was shown not to be subject to hexose-mediated repression during mixed sugars fermentation. PTD3 produced ethanol of 84% of theoretical during fermentation of glucose. It produced considerable amount of xylitol of 67% of theoretical when xylose was present in the fermentation media. This novel yeast has also a high tolerance of inhibitors (furfural, 5-hydroxymethylfurfural (5-HMF) and acetic acid) during biological production of ethanol and xylitol. PTD3 can effectively ferment five and six carbon sugars present in hydrolyzates from different cellulosic biomass (steam pretreated switchgrass, mixture of hardwoods and softwoods and sugar cane bagasse) to xylitol and ethanol.

David Keffer, University of Tennessee

Nanoscale Membrane Design Principles for Optimizing Proton Conductivity

A model for charge transport in aqueous systems is used to provide insights into design of proton exchange membranes that optimize charge transport. The model accounts for the effect of acidity, confinement and connectivity on the diffusivity and has been shown to quantitatively agree with experimental measurements of charge self-diffusivity in Nafion [Esai Selvan, M., et al. *J. Phys. Chem. B* **115** 2011 pp 3052–3061] and in cross-linked and sulfonated polycyclohexadiene. In this presentation, the origin of the theoretical model is described. The model is applied to water-filled cylindrical nanopores functionalized on their interior surface with acid groups. It is demonstrated that for cylindrical nanopores of a given radius there is an optimal surface coverage of acid groups. The optimum can be sharply peaked, indicating that non-optimal surface coverages (either too low or too high) drastically reduce the conductivity of the pore. The theoretical maximum conductivity through a cylindrical nanopore is calculated to be about 0.70 S/cm at 300 K. Comparison with available experimental results is made. Limitations of the model are also discussed.

Peter Pfromm Kansas State University

Fuels and chemicals from biomass in the central plains: Will farmers grow the crop for us, and how do we process it?

Patrick Bollin, PhD Student and IGERT Trainee, IGERT IStar BioEnergy, Department of Chemical Engineering, Kansas State University, Manhattan, Kansas

Jason Fewell, PhD Student and IGERT Trainee, IGERT IStar BioEnergy, Department of Agricultural Economics, Kansas State University, Manhattan, Kansas

Dr. Mary E. Rezac (PI), Dr. Peter H. Pfromm (co-PI, presenter), IGERT IStar BioEnergy, Department of Chemical Engineering, Kansas State University, Manhattan, Kansas

The technological and end-use market aspects of crop-based bioenergy often dominate the discussion, our research directions, and public investments. The most fundamental and arguably most crucial issue, however, is the willingness of farmers to produce the raw materials with long-term commitments geographically close to the processing facilities. Here, a socio-economic study was performed to investigate if farmers can be motivated to consistently provide the irreplaceable biomass. The thresholds for costs, personal engagement, and motivation were probed by collecting extremely valuable primary data in face-to-face interviews with a statistically significant number of Kansas farmers. While the supply of biomass is absolutely crucial, many roadblocks in the technical area also need to be removed. Fast pyrolysis of biomass to bio-oil has been selected by some research groups and companies as the optimum path to liquid fuels and chemicals. However, the high oxygen content of pyrolysis oil is generally recognized as problematic and needs to be reduced to increase stability and processing options. We show a reactive membrane approach to hydrotreating for deoxygenation of bio oil at 2 atmospheres of hydrogen and below 100C, as opposed to the current state of the art that requires on the order of 50 atmospheres of hydrogen and up to 400C.

Ajay K. Prasad University of Delaware

Sustainable Energy from Solar Hydrogen: Development of a Novel Ultra-High Temperature Thermochemical Reactor for Solar Energy Harvesting and Fuel Production

Erik Koepf, IGERT Trainee, Ph.D. Candidate, Advisors: Dr. Suresh G. Advani, Dr. Ajay K. Prasad
Program PI: Dr. Robert Opila

The large scale harvesting and storage of solar energy in chemical form, or the creation of solar-fuels, is a promising component of a sustainable energy future. One such application of this approach is water-splitting by ultra-high temperature thermochemical cycles. A solar-thermochemical reactor design and demonstration project has been underway at the University of Delaware since 2007. We have contributed significantly to the field of concentrated power-tower solar-thermal fuels in the areas of receiver/reactor design, ultra-high temperature solar-thermal solid-particle decomposition modeling, vortex flow generation and visualization, and reactant feed mechanisms. Our novel receiver/reactor design features a cavity-type reaction environment with continuous or batch reactant feeding and controlled residence time through engineered temperature zones. Reactant ZnO powder is gravity-fed annularly from above and highly concentrated solar radiation enters through a small aperture above. The use of a unique inverted cone-shape reactive surface, coupled with a controlled vortex flow, enables the reactant bulk-flow to cover the cavity surface area creating efficient energy conversion. Reactor testing is currently underway using the 10,000C-peak high-flux solar simulator at PSI, Zurich.

Ram Seshadri, University of California, Santa Barbara

Advances in the science and technology of phosphor converted solid state white lighting

Materials Department and Department of Chemistry & Biochemistry
Materials Research Laboratory
University of California, Santa Barbara CA 93106-5121

The ConvEne IGERT program seeks to holistically train graduate students from multiple disciplines in the science, engineering, economics, and policy aspects of energy conversion; a lot of the science focuses both on the conversion of light into electricity (solar photovoltaics) and on the conversion of electricity into light (light emitting diodes). Here we will discuss some of the research being carried out by IGERT graduate students, in this latter aspect of energy conversion, discussing the science and engineering of phosphor-converted solid state white lighting. In particular, on emphasis of using characterization techniques, drawn from distant fields, to better understand the source of phosphor efficiency will be discussed.

Cognitive, Social, and Economic Science

Eileen Kowler, Rutgers University

The perception of motion is vital to behavior, survival and communication. Interdisciplinary teams studied the perception and production of motion in virtual and real environments. One team (directed by J. Feldman) created artificial agents who explored, foraged or fought using intelligent decision rules. Observers could infer the agents' intentions on the basis of features of their motions. A second team (E. Torres) used motion-capture tools to record human actors performing complex activities (e.g., tennis serves). The group modeled the movements, and produced realistic percepts by endowing an animated avatar with the same models. A third team (E. Kowler) found that pursuit eye movements when viewing one's moving arm were evoked by signals derived from arm motor planning. Taken together, these results show remarkable overlap in the control of the perception and production of motion. This overlap facilitates the ability to perform complex motor tasks or to interpret motor patterns of others. Understanding connections between the perception and production of motion is crucial in fields ranging from the study of social interactions to the design of virtual environments.

Memon Nasir, New York University

The increasing popularity of Online Social Network sites, such as Facebook, and the information sharing by its users have privacy implications that are yet to be understood. Research studies and known examples demonstrate the fact that people under-estimate the risks in sharing information online. Specifically, users share too much information, Facebook does not adequately protect user privacy and third-parties actively seek information about Facebook users. Personality traits are believed to influence the use of social media and also have an effect on Internet security awareness. We examine how the traits affect Facebook-related decision making and behavior. The Big Five framework of personality traits (known as OCEAN – Openness, Conscientiousness, Extraversion, Agreeableness and Neuroticism) from Costa & McCrae has been identified as a robust model for understanding the relationship between personality and various academic behaviors. Our research sets to examine if this relationship extends to online privacy-related behavior. For example, we examine how Neuroticism affects the way users set their privacy settings on Facebook and whether it is related to higher security awareness. On the other hand, we check if Extraversion and Openness predict how much information users will share online. Another aspect we plan to examine relates to phishing attacks. Phishing attacks are a way of attempting to get personal information from users and represent a form of social engineering techniques used to deceive users. Previous research showed a success rate of up to 70% for phishing attacks on social networks. We will look at the correlation between deception detection and personality traits, and how it affects the likelihood of falling for an email phishing attack. We conduct a study with about a 100 users to determine these correlations and how they can be used to help predict privacy-related online behavior. We believe that better understanding of the reasons for online vulnerability can help prevent such behavior and increase users privacy and security in the future.

Computation, Sensing, and Devices

Silvia Ferrari, Duke University

Information-driven Modeling and Control of Mobile Sensor Networks

Unmanned ground, aerial, and underwater vehicles equipped with on-board wireless sensors are becoming crucial to both civilian and military applications because of their ability to replace or assist humans in carrying out dangerous yet vital missions. As they are often required to operate in unstructured and uncertain environments, these mobile sensor networks must be adaptive and reconfigurable, and decide future actions intelligently based on the sensor measurements and environmental information. In particular, our recent work on geometric path planning has shown that the sensing performance of these sensors can be significantly improved by planning their paths based on probabilistic sensor models, and on the geometric characteristics of the workspace and of the sensors' fields-of-view. This talk presents new methods based on computational geometry and optimal control that can be used for planning the paths of mobile sensors in order to optimize their ability to monitor, classify, and model their environment. A novel framework is presented that combines Bayesian probability, information theory, and computational geometry to automate and optimize the management of information-gathering agents. This framework has been demonstrated through numerous sensor applications such as demining, undersea surveillance, and games. This talk will show how the approach has been recently extended to multi-scale sensor networks, involving hundreds of agents. Also, it will discuss emerging applications, such as, the geospatial monitoring of air quality and pollutants, and the monitoring of landfills, and oil and gas production through the detection of leaks over large areas using unmanned ground vehicles equipped with onboard instrumentation for *in-situ* sensing and data analysis.

Falko Kuester, University of California, San Diego

CyberArchaeology: Creating a Future for the Past

Pollution, natural disasters, theft, fatigue, overexposure, mismanagement, and the unintended consequences of existing efforts to preserve our cultural patrimony have all taken a major toll on our built infrastructure as well as sculptures, paintings, archaeological and other artifacts that constitute our cultural heritage. Science, engineering and the arts offer the best hope for improving stewardship of these cultural assets and reversing decades or even centuries of damage. New methodologies and techniques for cultural heritage diagnostics and preservation are therefore needed, including diagnostic and analytical imaging as well as visual and cultural analytics in collaborative digital workspaces that provide engineers, scientists, art historians and restorers, with a means to intuitively and interactively explore historic artifacts. IGERT-TEECH research is creating the foundation for the next generation of cyber-archaeology that will provide a means to researchers and the public alike to study cultural heritage and facilitate its preservation. This talk will outline our cyber-archaeology approach anchored in science and engineering and its application to three unique case study environments in Italy, Jordan and Mongolia.

Mike Mooney, Colorado School of Mines

Towards Intelligent Earth Dams and Levees

Nearly 200,000 kilometers of earthen levees and 100,000 earthen dams in the U.S. collectively provide flood protection, water supply and renewable energy for hundreds of millions of Americans. This vast network of earth dams and levees (EDL) in the U.S. and worldwide (e.g., Netherlands is protected by 17,000 km of levees, aka dikes) is human-made; we have re-shaped the earth to permit our way of life. The role of EDLs in society grows with time as people continue to urbanize to cities and coastal areas protected by human-made earthen structures, as storm events increase and as sea levels rise. This presentation will summarize an integrative, interdisciplinary approach to characterizing the health, behavior and risk of this vast network of EDLs through an intelligent geosystems approach. Students and faculty from 6 disciplines: civil engineering, mechanical engineering, computer science, geophysics, geology and public policy are working in collaborative research teams to advance global (via satellite remote sensing) to local (via laboratory ultrasonic imaging of grains) monitoring of earth dam and levee behavior. Researchers are working across these disciplines to identify signs of weakness across

Sethuraman Panchanathan, Arizona State University

Recent years have witnessed an increased emphasis on the need for human-centeredness in multimedia computing. In contrast to existing approaches that rely on the so-called “able” population, we have proposed a new archetype to human-centered multimedia computing inspired by technology solutions for individuals with disabilities. The study of sensory, motor, perceptual and cognitive disabilities has helped us understand the subtleties of human capabilities and limitations, thus guiding the design of newer methodologies for data sensing, processing and delivery. At the Center for Cognitive Ubiquitous Computing at Arizona State University, we employ an interdisciplinary research approach, involving computer scientists, cognitive psychologists, design engineers and community experts, for the design and development of innovative multimedia solutions that not only enrich the lives of individuals with disabilities, but also address the needs of a broader community of users. This unique paradigm of multimedia computing will be illustrated through two case studies: the NoteTaker, a device to assist low-vision students in classroom note-taking, and the Social Interaction Assistant, a suite of technologies to enrich the experience of social interactions for the visually impaired.

Cynthia Peterson, University of Tennessee

Discovery of new pharmaceuticals is costly and time consuming, and research can quickly become a needle-in-a-haystack effort. Virtual screening can greatly reduce cost and time and also significantly increase potential search space to increase chances of finding a novel compound. This research aims to develop a supercomputing-based research tool based on validated and widely used docking approaches adapted for high-throughput screening of millions of compounds in a single day. Existing programs are adapted to use a Message Passing Interface (MPI) protocol to enable parallel computations of a target protein on thousands of processors simultaneously via massively parallel architectures. Virtual screening can now be run on over 65,000 processors in parallel on a supercomputer and essentially achieve in a day what used to take several weeks. These same tools can also be used to facilitate and expedite screening of prospective pharmaceuticals for toxicity and side effects. Importantly, this technological advance also allows the research community to simulate complex scenarios in cells containing multiple binding proteins, expanding isolated virtual in-vitro binding tests to multi-component virtual cell-based assays.

Rafael Piestun, University of Colorado at Boulder

Computational Optical Sensing and Imaging A new paradigm to overcome physical limits

We are witnessing the emergence of a new paradigm of sensing and imaging, where an integration of fundamental scientific discoveries (e.g. quantum optics, compressive sensing) and technological impetus (e.g. sensor arrays, nanostructures) creates functional systems that greatly overcome the simple superposition of the parts. Abbe's resolution limit has been overcome after more than 130 years enabling unprecedented opportunities for optical imaging at the nanoscale. Now, fluorescence imaging using photoactivatable/photoswitchable molecules within computational optical systems offers single molecule sensitivity. Point spread function engineering matched with reconstruction algorithms enables super-resolution in three dimensions to reveal deep sub-cellular structure. Focusing and imaging through strongly scattering media has also been accomplished recently in the optical regime. Wavefronts overcome the effects of multiple scattering by using a feedback system and optical modulation. In particular, a phase-control holographic technique helps characterize the scattering media at high speed using micro-electro-mechanical technology, allowing focusing through a temporally dynamic scattering sample.

Mike Evans on behalf of Shashi Shekhar, University of Minnesota

Eco-routes aim to minimize fuel consumption and green-house gas emission (rather than travel-time or distance) via avoiding congestion, idling at red-lights, turns and elevation changes, etc. For example, large fleet owners, e.g. UPS, save millions of gallons of fuel per year by avoiding routes with left turns and associated idling. Some believe that appropriately designed Eco-Routes and related navigation services leveraging historic and real-time traffic information may save consumers hundreds of Billions of dollars in coming decade. A few navigation devices (also known as GPS devices) recently introduced Eco-Route options, though consumer experience is mixed and many questions are not addressed:

- What are expected fuel saving from use of GPS devices with static roadmaps?
- What the value-added by historical traffic and congestion information?
- How much additional value is added by real-time traffic information?
- What is computational structure of the determining routes that minimize fuel consumption and green-house gas emissions?
- Does this problem satisfy the assumptions behind common shortest-path algorithms?

This talk will explore some of these questions.

Venkatakrishnan Venkatesan, University of Illinois at Chicago

Online Advertising: Security, Privacy Risks and Mitigations

Users of the World Wide Web routinely encounter online advertisements that pose severe security and privacy risks. At the one end of the spectrum are security risks from malicious actors that employ rogue advertisements that often escape existing weak defenses employed by ad networks and websites, inflicting much harm on end-users. On the other end of the spectrum are privacy risks from behavioral advertising in which business entities that aim to tailor web advertising as closely possible to an individual's interests, resulting in loss of control over personal information. These security and privacy risks have led to a crisis in online advertising, which is exacerbated by several factors: complex mechanisms by which web ads are produced, distributed and deployed; weak filtering strategies of ad networks; poor technical solutions for ad isolation and confinement; lack of effective technologies or regulations to prevent third party tracking and the lack of incentives in the advertising ecosystem to adopt less privacy invasive practices. We describe the research being done in the Electronic Security and Privacy IGERT in developing norms for advertising frameworks that allow users to avoid these security and privacy risks while benefitting from the advantages of secure information processing that include increased availability of relevant information, increased economic efficiency, improved security, and personalization of services.