Interdisciplinary Symposium on Advanced Nano/Biosystems: Design, Fabrication, and Characterization

September 25-27, 2013

Materials Research Lab
Room ESB190
University of Illinois
Urbana, Illinois

BECKMAN INSTITUTE
FOR ADVANCED SCIENCE AND TECHNOLOGY

Interdisciplinary Symposium on Advanced Nano/Biosystems: Design, Fabrication, and Characterization

September 25-27, 2013
Materials Research Lab, Room ESB190
University of Illinois at Urbana-Champaign

SYMPOSIUM SCHEDULE Room ESB190

Wednesday, September 25

8-9 a.m. **Breakfast**

9-10 a.m. **Klaus Schulten**
Computational Microscopy for Health and Technology

SESSION 1
Multiscale modeling and computation of advanced materials and structures

Session chair *Horacio Dante Espinosa*

10-10:30 a.m. **Aleksei Aksimentiev**
Nanopore Sequencing of DNA

10:30-11 a.m. **Katherine Yanhang Zhang**
Contributions of Collagen and Elastin to the Mechanobiology of Arteries

11-11:20 a.m **Coffee break**

SESSION 2
Design and fabrication of multifunctional nano/biomaterial system

Session chair *Horacio Dante Espinosa*

11:20-11:50 a.m. **Guy Genin**
The Spectacular Nano-Structured Attachment of Tendon to Bone and Our Appalling Attempts to Reconstitute It

11:50-12:20 p.m. **Mark Bathe**
Rational Design of MegaDalton-Scale DNA-Based Light Harvesting Antennas

12:20-2 p.m. **Lunch**
201 MRL

SESSION 3

Self-assembly of bio/nanomolecules and particles

Session chair *Katherine Yanhang Zhang*

2-2:30 p.m. **Peng Yin**
Programming Nucleic Acids Self-Assembly

2:30-3 p.m. **Xi Chen**
Mechanical Self-Assembly

3-3:30 p.m. **William Wilson**
Excited State Dynamics of Flow-assembled Synthetic Pi-Core Polypeptides: A FLIM Study of Exciton Relaxation in Aligned Bio-Organic Nanomaterials

3:30-3:50 p.m. **Coffee break**

SESSION 4

One-dimensional nanostructured materials and devices

Session chair *SungWoo Nam*

3:50-4:20 p.m. **M. Samy El-Shall**
Metal and Semiconductor Nanoparticles Supported on Graphene for Energy Conversion and Heterogeneous Catalysis

4:20-4:50 p.m. **SungWoo Nam**
All-Carbon Graphene Bioelectronics

4:50-5:20 p.m. **Sriraam Chandrasekaran**
Graphene Synthesis from Biochar using Wet Chemical Treatment Process

Thursday, September 26

8-9 a.m. **Breakfast**

9-10 a.m. **John A. Rogers**
Stretchy Electronics That Can Dissolve in Your Body

SESSION 5
Multifunctional micro/nanofluidic structures and devices

Session chair *Wayne Chen*

10-10:30 a.m. **Horacio Dante Espinosa**
Fluidic Nanoprobes for *in vitro* Single Cell Studies

10:30-11 a.m. **Narayana Aluru**
TBA

11-11:20 a.m. **Coffee break**

SESSION 6
Mechanics of advanced materials (functional/smart/energy/bio/nanomaterials)

Session chair *Wayne Chen*

11:20-11:50 p.m. **Xiaodong Li**
Structural Origin of Flaw Tolerance in Nacre

11:50-12:20 p.m. **Nikhil Koratkar**
Wetting Translucency of Graphene

12:20-2 p.m. **Lunch**
201 MRL

SESSION 7

Bio-inspired design and fabrication of actuator/sensor/gate/switch

Session chair *Xiaodong Li*

2-2:30 p.m. **Jean-Pierre Leburton**
Multi-Function Semiconductor Membranes with Nanopore for Bio-Molecule Sensing and Manipulation

2:30-3 p.m. **Wanliang Shan**
Bioinspired Design of Wearable Device with Electrically Tunable Rigidity

3-3:30 p.m. **Yulia Maximenko**
Microcapsules for Luminescent Tracking and Controlled Drug Delivery

3:30-3:50 p.m. **Coffee break**

SESSION 8

Advanced mechanical testing and material analysis techniques

Session chair *Xiaodong Li*

3:50-4:20 p.m. **Wayne Chen**
Dynamic Mechanical Responses of Soft Biological Tissues

4:20-4:50 p.m. **Elizabeth Horstman**
A Microfluidic Approach for Cocrystallization of Drugs and Analysis via X-Ray Diffraction

4:50-5:20 p.m. **Zhao Qin**
Multi-Scale Modeling of Protein Materials and Their Mechanics

Friday, September 27

9-10:30 a.m. **Chaitanya Sathe**
An Introduction to Computational Modeling using VMD and NAMD

10:30-11 a.m. **Break**

11-12:30 p.m. **Maxim Belkin**
Overview of Advanced NAMD Features and Their Application in Simulations

12:30-2 p.m. **Lunch**
201 MRL

2-4 p.m. **Tour of experimental facilities at MRL**

Thank you for attending!

If you should have any questions or concerns, please do not hesitate to contact the symposium co-chairs:
Baoxing Xu: 646-509-7368
Ilia Solov'yov: 217-979-9613

Organization Committee:

Ilia Solov'yov (co-chair)
Baoxing Xu (co-chair)
Patricia Jones
Maeve Reilly
Jordan Lowe
Chris Johns
Susan Lighty
William Wilson

This conference is sponsored in part by the Beckman Institute for Advanced Science and Technology and the Frederick Seitz Materials Research Laboratory.

Wednesday Keynote Speaker: KLAUS SCHULTEN, 9 a.m.

Klaus Schulten received his Ph.D. from Harvard University in 1974. He is a Swanlund Professor of Physics and is also affiliated with the Department of Chemistry as well as with the Center for Biophysics and Computational Biology. Professor Schulten is a full-time faculty member at the Beckman Institute and directs the Theoretical and Computational Biophysics Group. His professional interests are theoretical physics and theoretical biology. His current research focuses on the structure and function of supramolecular systems in the living cell, and on the development of non-equilibrium statistical mechanical descriptions and efficient computing tools for structural biology.

Computational Microscopy for Health and Technology

It is today becoming possible to view and study biological systems on the cellular scale using computational methods, offering insights into new solutions to mankind's health and energy needs. Engineers and scientists at our NIH Center for Macromolecular Modeling and Bioinformatics have worked over the last two decades to combine the most advanced computer technology and the best biomedical science to develop a suite of computer programs that today serve more than 300,000 registered users in many fields of biology and medicine. These programs utilize the most highly resolved microscopies (x-ray, electron beams) to provide chemically detailed views of systems such as healthy and diseased cells and of whole viruses.

Our center recently published the first complete atomic resolution structure of the full HIV capsid; this structure is already being used to help understand how HIV-inhibiting drugs work on the capsid, thus offering unprecedented opportunities for developing pharmacological interventions. Our center also studies, at the most detailed level possible, the chemical processes involved in second-generation biofuels production and in photosynthesis to help guide new means of extracting chemical energy from renewable resources. We will soon be able to generate atomic-level views of entire living cells, opening a treasure chest of data for biotechnology, pharmacology, and medicine.

This lecture will present practical applications of computational microscopy covering nanosensor development, protein design, antibiotics, antiviral drugs, photosynthesis, and novel enzymes for producing biofuels from agricultural waste.

Thursday Keynote Speaker: JOHN A. ROGERS, 9 a.m.

John Rogers received B.A. and B.S. degrees in chemistry and in physics from the University of Texas, Austin, in 1989. He earned S.M. degrees in physics and in chemistry in 1992, and a Ph.D. degree in physical chemistry in 1995, all from MIT. In 1997, he joined the Department of Condensed Matter Physics Research at Bell Laboratories. From 2000-2002 he served as director of that department. He is currently a Founder Professor of Engineering in the University of Illinois departments of Materials Science and Engineering and of Chemistry. He is a full-time faculty member in the 3D Micro- and Nanosystems Group at the Beckman Institute. His research interests are in the science and engineering of unconventional, "soft" materials—polymers, small molecules, fluids, carbon nanotubes—and in the development of unusual ways for patterning them with micron and nanometer resolution—printing, molding, and near field photolithography.

Stretchy Electronics That Can Dissolve in Your Body

Biology is soft, curvilinear, and transient; modern silicon technology is rigid, planar, and everlasting. Electronic systems that eliminate this profound mismatch in properties will lead to new types of devices, capable of integrating noninvasively with the body, providing function over some useful period of time, and then dissolving into surrounding biofluids. Recent work establishes a complete set of materials, mechanics designs, and manufacturing approaches that enable these features in a class of electronics with performance comparable to that of conventional wafer-based technologies. This talk summarizes the key ideas through demonstrations in skin-mounted "epidermal" monitors, advanced surgical tools, and bioresorbable electronic bacteriocides.

BIOGRAPHIES & ABSTRACTS

SESSION 1 – 10 a.m., Wed., Sept. 25

Aleksei Aksimentiev (University of Illinois at Urbana-Champaign) received his master's degree in physics from the Ivan Franko Lviv State University, Lviv, Ukraine, and his Ph.D. in chemistry from the Institute of Physical Chemistry, Warsaw, Poland. After a brief postdoctoral training at Mitsui Chemicals, Japan, he joined the Theoretical and Computational Biophysics Group as a postdoctoral research associate. In 2005, he became a faculty member of the Physics Department at the University of Illinois, where he is currently an associate professor of physics. His research interests include systems that combine biological macromolecules and man-made nanostructures, membrane proteins, and molecular machinery of DNA replication.

Nanopore Sequencing of DNA

The idea of using a nanopore to sequence DNA continues to generate excitement among scientists and entrepreneurs. The spectacular progress in using biological enzymes to enable nanopore sequencing indicates the imminent arrival of nanopores in practical biomedical applications. Even more exciting are the prospects of creating solid-state devices that can read the nucleotide sequence directly from DNA and RNA molecules. In this talk I will describe our recent efforts to model such devices at atomic resolution and develop strategies for electronic readout of the DNA sequence.

Katherine Yanhang Zhang (Boston University) is an associate professor in the Departments of Mechanical and Biomedical Engineering and director of the Multi-Scale Tissue Biomechanics Laboratory at Boston University. Dr. Zhang received her B.S. degree in engineering mechanics from Tsinghua University, China in 1998; and M.S. and Ph.D. degrees in mechanical engineering from University of Colorado at Boulder in 2000 and 2003. She was a Clare Boothe Luce Assistant Professor of Boston University from 2006-2011. Dr. Zhang's research has focused on multi-scale mechanics and mechanobiology of extracellular matrix and vasculature. She is the recipient of prestigious Faculty Early Career Development (CAREER) Award from NSF in 2010, and Young Faculty Award from DARPA in 2007.

Contributions of Collagen and Elastin to the Mechanobiology of Arteries

Cardiovascular diseases (CVDs) are the leading cause of death in the Western world. It is responsible for 40 percent of all the deaths in the United States, more than all forms of cancer combined. While CVDs is a broad term used to describe a range of diseases that affect heart and blood vessels, arteriosclerosis or hardening of the arteries is presented in many of these diseases. The extracellular matrix (ECM) of the aortic wall plays an important role in the pathogenesis of arteriosclerosis, aortic aneurysms, etc. The aortic wall is largely composed of fibrous materials, collagen, and elastin, and ground substance interspersed among organized layers of cells to form lamellar structures. The prevailing concept is that elastin and collagen are the primary load-bearing components of vascular tissue, respectively, in low-stretch or high-stretch regions of stress-strain curves. In this work we investigated the interactions among these ECM constituents and how they affect vascular function. A microstructural-based constitutive model was developed to incorporate the structural information such as fiber orientation, undulation distributions, and fiber density in describing the aortic mechanical response. Study of structural changes during normal stretching as well as elastin degradation was performed with second harmonic generation and two photon excitation fluorescence imaging. Together these results provide a more comprehensive study of the structure function relationship with the goal of incorporating this information in understanding disease progressions and structurally based constitutive models.

SESSION 2 – 11:20 a.m., Wed., Sept. 25

Guy Genin (Washington University at St. Louis) received B.S.C.E. and M.S. degrees in engineering mechanics from Case Western Reserve University in 1992, and S.M. and Ph.D. degrees in applied and solid mechanics from Harvard University in 1993 and 1996, and postdoctoral training at Cambridge and Brown. He is a professor of mechanical engineering and materials science at Washington University, and of neurological surgery at Washington University School of Medicine. His professional interests involve study of interfaces and adhesion in physiology, nature, and engineering. His current research focuses on connections between tendon and bone, and on interactions between plant and animal cells with their mechano-electric environment.

The Spectacular Nano-Structured Attachment of Tendon to Bone and Our Appalling Attempts to Reconstitute It

Joining mechanically dissimilar materials is a challenge throughout engineering, with spectacular and often devastating failures. This challenge also underlies one of the worst procedures in all of medical practice, the surgical reattachment of tendon to bone. The body presents a highly effective attachment prior to injury, but the tissue regenerated following healing is vastly inferior mechanically and surgical outcomes can be abject failures, with recurrence of tears as high as 94 percent following surgical repair of massive rotator cuff tears in elderly patients.

Our group studies how the natural tendon-to-bone attachment develops, functions, and heals, and how healing might be improved through tissue engineered augmentation. Although much of the basic physiology is still debated, it is clear that choreographed, nanoscale-to-milliscale toughening mechanisms are at play, and that mechanical factors play a central role in developing and sustaining these mechanisms. Hierarchical toughening mechanisms involve tailoring of the collagen lattice upon which the entire tendon-to-bone attachment is constructed, and accommodation by this lattice of a relatively stiff hydroxyl apatite phase. Toughening strategies include cross-scale functional grading of the mineral component within collagen, macro-scale interdigitation of bony and tendinous tissue, and shape optimization to distribute stresses.

Central challenges are understanding how mineral accumulates on the collagen lattice underlying tendon, bone, and its connection, and quantifying the mechanical consequences of adding prescribed amounts of mineral, both to this collagen lattice and to potential scaffolds for guiding healing. This talk will focus on our recent efforts to characterize and reconstitute the nano-to-milliscale physiology of the tendon-to-bone attachment at the humeral head of the rotator cuff.

Mark Bathe (MIT) is an assistant professor in the Department of Biological Engineering at MIT with a joint appointment in the Department of Mechanical Engineering. He received his B.S., M.S., and Ph.D. degrees from MIT in 1998, 2001, and 2004, respectively, in the Department of Mechanical Engineering. He directs the Laboratory for Computational Biology and Biophysics that seeks to develop innovative computational tools to enable the rational forward design of synthetic biological components based on structural DNA nanotechnology, and Bayesian approaches to reverse engineer dynamic biological processes from fluorescence imaging and spectroscopy data.

Rational Design of MegaDalton-Scale DNA-Based Light Harvesting Antennas

Programmed self-assembly of DNA using scaffolded DNA origami offers the unique opportunity to engineer complex structural assemblies at the MegaDalton-scale with sub-nanometer precision. Due to their sequence specificity, these nucleic acid assemblies also serve as programmable structural scaffolds to host secondary, light-harvesting molecules and thereby serve as biomimetic light-harvesting antennas for artificial photosynthesis. Here, I present our computational design tool CanDo (cando-dna-origami.org) that predicts both the overall 3D architecture of MegaDalton-scale DNA-based assemblies as well as their light-harvesting properties when used as scaffolds to host chromophores and porphyrins. This computational design framework enables the rapid in silico design and evaluation of functional light-harvesting constructs to mimic bacterial light-harvesting assemblies.

SESSION 3 – 2 p.m., Wed., Sept. 25

Peng Yin (Harvard) is an assistant professor in the Department of Systems Biology at Harvard Medical School and a core faculty member at the Wyss Institute for Biologically Inspired Engineering at Harvard. He received his B.S. in biochemistry and molecular biology, and bachelor of economics from Peking University in 1998; and his M.S. in molecular cancer biology and Ph.D. in computer science from Duke University in 2000 and 2005, respectively. His research interests lie at the interface of information science, molecular engineering, and biology. The current focus is to engineer information directed self-assembly of nucleic acid (DNA/RNA) structures and devices, and to exploit such systems to do useful molecular work, e.g., probing and programming biological processes for bioimaging and therapeutic applications.

Programming Nucleic Acids Self-Assembly

I will discuss my lab's (molsys.net) research on engineering synthetic, nucleic acid-based nanostructures and applications. We have recently invented a general framework for programming the self-assembly of short synthetic nucleic acid strands into prescribed target shapes or demonstrating their prescribed dynamic behavior. Using short DNA strands, we have demonstrated the modular construction of sophisticated 2D and 3D structures on the 100-nanometer scale with nanometer precision. Using

reconfigurable DNA hairpins, we have demonstrated diverse, dynamic behavior such as catalytic circuits, triggered assembly, and autonomous locomotion. By interfacing these synthetic, nucleic acid nanostructures with functional molecules, we are developing a diverse range of applications. In biosensing, we have constructed robust and specific probes for detecting single-base changes in a single-stranded DNA/RNA target. In bioimaging, we have engineered geometrically encoded fluorescent barcodes for highly multiplexed single-molecule imaging. In nanofabrication, we have developed a versatile framework for producing inorganic materials (e.g., graphene, silicon dioxide, silver, and gold) with arbitrarily prescribed nanometer scale shapes. Finally, I'll discuss our ongoing work to move the nanostructures from test tubes to living cells.

Xi Chen (Columbia University) received his Ph.D. in solid mechanics from Harvard University in 2001 and was a postdoc from 2001-2003. He has been with Columbia University since 2003 and currently an associate professor with tenure. He uses multiscale theoretical, experimental, and numerical approaches to investigate various research frontiers in materials addressing challenges in energy and environment, nanomechanics, and mechanobiology. He received the NSF CAREER Award in 2007, the Presidential Early Career Award for Scientists and Engineers (PECASE) in 2008, ASME Sia Nemat-Nasser Early Career Award in 2010, SES Young Investigator Medal in 2011, and ASME Thomas J. R. Hughes Young Investigator Award in 2012. He is also a Changjiang Chair Professor of China.

Mechanical Self-Assembly

Numerous highly ordered patterns can be achieved by manipulating the self-assembled buckling of thin films on compliant substrates upon mismatched deformation. Most previous studies were limited to planar substrates, and the investigation of a closed film on a curved substrate is rare yet such a system is highly relevant to quite a few natural and biological systems. We establish the framework of elastic buckling of a model spheroidal thin film/substrate system, in which the bifurcation is driven by anisotropic (non-equi-biaxial) compressive stresses in the film. A reduced theoretical model is proposed, from which explicit formulae are derived to correlate the undulation characteristics with the geometry and material property of a prolate system. Various ways to manipulate the undulations are discussed. It is shown that some global features of quite a few natural and biological systems, for example the distinctive patterns observed in various fruits, vegetables, nuts, eggs, tissues, animal body parts, etc., can be reproduced by anisotropic stress-driven buckling on spheroidal film/substrate models. The mechanical principles and the potential of mechanical self-assembly

are demonstrated for fabricating 3D gear-like microstructures. Thus, the mechanics framework studied herein has important implications on morphogenesis, as well as having potential applications to guide micro-fabrications via controlled self-assembly on curved substrate surfaces.

William Wilson (University of Illinois at Urbana-Champaign)

Excited State Dynamics of Flow-Assembled Synthetic Pi-Core Polypeptides: A FLIM Study of Exciton Relaxation in Aligned Bio-Organic Nanomaterials

We have used hydrodynamic flow-driven assembly of synthetic peptides in microfluidic reactors to generate a new class of functional materials. This strategy is highly repeatable and allows for compositional and structural control over the assembled media. Microfluidic-driven assembly is carried out in a rapid, scheduled format on-chip that offers the potential for fabrication scalability. We explore an integrated molecular-level understanding of these engineered systems using spatially resolved spectral tools. In this system example, exciton dynamics in engineered H-aggregate polypeptides is discussed.

SESSION 4 – 3:50 p.m., Wed., Sept. 25

M. Samy El-Shall (Virginia Commonwealth University) is a professor of chemistry and chemical engineering at Virginia Commonwealth University (VCU). He received his B.S. and M.S. degrees from Cairo University, and a Ph.D. from Georgetown University. He did postdoctoral research in nucleation and clusters at UCLA. His research interests are in the general areas of molecular clusters, nucleation phenomena, nanostructured materials, and graphene and nanocatalysis for energy and environmental applications. He has published more than 210 refereed papers and review chapters, and he holds eight U.S. patents on the synthesis of nanomaterials, nanoalloys, nanoparticle catalysts, graphene, and graphene-supported catalysts. Dr. El-Shall received the Outstanding Faculty Award of Virginia in 1999; the Distinguished Research Award from the Virginia Section of the American Chemical Society in 2009; the Innovative Research Award from the Society of Automotive Engineering (SAE) in 2009; and the VCU Distinguished Scholarship Award in 2011. He was elected as a Fellow of the American Physical Society in 2012, and was selected as a Jefferson Science Fellow at the U.S. Department of State for 2012-2013.

Metal and Semiconductor Nanoparticles Supported on Graphene for Energy Conversion and Heterogeneous Catalysis

Graphene has attracted great interest for a fundamental understanding of its unique structural and electronic properties and also for important potential applications in nanoelectronics and devices. The combination of highest mobility, thermal, chemical, and mechanical stability with the high surface area offers many interesting applications in a wide range of fields including heterogeneous catalysis where metallic and bimetallic nanoparticle catalysts can be efficiently dispersed on the graphene sheets.

We have developed facile and scalable chemical and physical reduction methods for the synthesis of chemically and laser converted graphene, as well as for metal and semiconductor nanoparticles dispersed on graphene. This talk will address two novel aspects of graphene research dealing with the efficient photothermal energy conversion by graphene and nanocatalysis by metal-graphene nanocomposites. In the first aspect, the observed photothermal effects leading to a significant increase in the temperature of the solution suggests that metal-graphene nanocomposites could be promising materials for the efficient conversion of solar energy into usable heat for a variety of thermal, thermochemical, and thermomechanical applications.

In the second aspect, we demonstrate the excellent catalytic activity of Pd-graphene nanocomposites for the carbon-carbon Suzuki and Heck cross coupling reactions. These reactions have been extensively used for the assembly of complex organic molecules for a wide variety of applications with considerable impact on the chemical and pharmaceutical industries. The exceptional activity and stability of the Pd-graphene catalyst and the development of other novel metallic and bimetallic catalysts supported on graphene will be discussed.

Finally, we will present the application of graphene as a catalyst support for the Fischer-Tropsch Synthesis (FTS), which is increasingly attracting global interests as a consequence of environmental demands, technological developments, and changes in fossil energy reserves. The simultaneous chemical reduction of the metal precursors and graphene oxide in water under microwave irradiation allows the deposition of well-dispersed metal nanoparticles on the defect sites of the graphene nanosheets. The Fe-K-graphene catalyst exhibits high activity and selectivity towards higher products with excellent stability and recyclability. The exceptional activity and stability of the FTS-graphene catalysts will be presented and discussed.

SungWoo Nam (University of Illinois at Urbana-Champaign)

All-Carbon Graphene Bioelectronics

We report nano field-effect transistor (nanoFET) biosensors built from the monolithic integration of graphene and graphite. The monolithic integration enables nanoscopic field-effect detection of chemical and biological signals with mechanically flexible and robust interfaces with biological systems in several respects. Our nanoFET biosensors exhibit superior detection sensitivity, mechanical flexibility, and nanoscopic detection resolution. First, we demonstrate that electrical detection can be achieved from nanoscale electric field modulation of the graphene channel while the signal integrity is not perturbed by mechanical deflection of graphene nanoFET sensors. Such a capability is introduced by the advanced design of monolithic graphene-graphite without any need for metal-graphene heterointerfaces. Second, we explore the chemical detection capability of graphene nanoFET sensors, and show that our sensors are responsive to localized chemical environmental changes/perturbations. Our nanoFET sensors not only show clear response to nanoscopic charge perturbation but also demonstrate potential 3D sensing capability due to the advanced monolithic graphene-graphite mechanical design. These unique capabilities of our monolithic graphene-graphite bioelectronics could be exploited in chemical and biological detection and conformal interface with biological systems in the future.

Sriraam Chandrasekaran (University of Illinois at Urbana-Champaign)

Graphene Synthesis from Biochar using Wet Chemical Treatment Process

Biochar is a major by-product from pyrolysis and gasification of biomass. Biochar finds potential applications in soil amendment, carbon sequestration, super capacitors, adsorbents, etc. However, its applicability is limited by its properties such as low carbon content, low porosity, and surface area. Ongoing research on biochar explores thermal and chemical treatment to utilize the biochar in an effective way. This study focuses on converting the biochar to graphene-like thin films using a wet chemical process. Graphene is known for its potential applications as nanocomposites, electronic circuits, solar cells, and many other fields including medical, chemical, and industrial processes. The biochar prepared will be subjected to a pretreatment process, first oxidizing and subsequently reducing the strongly oxidized material. Although there are a few studies that concentrated on converting black carbon to graphene or graphene-like films, the carbon content of the starting materials used in those studies was about 99 percent. The carbon content of the biochar ranges from 50 percent to 85 percent. Thus, it is more challenging to convert them to high-quality graphene-like films. At each stage of the conversion process the reactants, products, and the by-products will be characterized by appropriate techniques. The study will explore the potential applications of the synthesized graphene.

SESSION 5 – 10 a.m., Thurs., Sept. 26

Horacio Dante Espinosa (Northwestern University and iNfinitesimal LLC) is the James and Nancy Farley Professor of Mechanical Engineering and the director of the Theoretical and Applied Mechanics Program at the McCormick School of Engineering, Northwestern University. He is a foreign member of the European Academy of Sciences and Arts and of the Russian Academy of Engineering. He is also Fellow of the American Academy of Mechanics, the American Society of Mechanical Engineers, and the Society for Experimental Mechanics. He received two Young Investigator Awards, the NSF CAREER Award, and the Office of Naval Research Young Investigator Award in 1997. He also received the American Academy of Mechanics (AAM) 2002 Junior Award, the Society for Experimental Mechanics (SEM) 2005 HETENYI Award, the Society of Engineering Science (SES) 2007 Junior Medal, and the 2008 LAZAN and 2103 Sia Nemat Nasser medals from the Society for Experimental Mechanics. He was the 2012 president of the Society of Engineering Science.

Professor Espinosa is also the founder and chief scientific officer of iNfinitesimal LLC, a nanotechnology company developing robust next-generation nanoscale devices, scalable nanomanufacturing tools, and microdevices for single cell transfection and analysis.

Fluidic Nanoprobes for *in vitro* Single Cell Studies

A robust method for single cell access to deliver genes and small molecules to primary and sensitive cells is needed to advance the state-of-the-art in personalized medicine and therapeutics. To realize this goal, a microfluidic chip, so-called nanofountain probes (NFP), has been developed for cell transfections using electric fields. The technology enables *in vitro* single-cell electroporation with very precise force and dosage control to achieve high cell viability. A localized electric field in the form of a square pulse with variable time duration is applied at the site of contact between probe and cell. This creates temporary pores on the cell membrane to facilitate dosage-controlled entry of biomolecules into the cytosol. To avoid excessive force on the cells and to increase viability after electroporation, the onset of probe-cell contact is detected using a change in the electrical resistance. Furthermore, dosage of the injected biomolecules into the cells is regulated through electric pulse duration. We have demonstrated NFP electroporation (NFP-E) of single HeLa cells within a population by transfecting them with fluorescently labeled dextran, green fluorescent protein (GFP) plasmids, proteins (BSA), and molecular beacons (DNA hairpins with fluorophores used to detect mRNA). Cells were imaged to evaluate the transfection

efficiency and cell viability. Moreover, theoretical analysis of the NFP-E delivery mechanisms revealed that application of an electric potential of a few hundred millivolts, between the NFP cantilevered tip and the region of the cell membrane in contact with the tip, creates nanopores in the cell membrane through which molecules diffuse to the cytoplasm. Experiments on HeLa cells confirmed that NFP-E offers single cell selectivity, high transfection efficiency (>95%), qualitative dosage control, and very high viability (92%) of transfected cells.

In this presentation, the advantages of NFP-based electroporation over other transfection and bulk electroporation techniques will be discussed. In particular, we will show results demonstrating precise molecular delivery while minimizing stress to the cell. The presentation will also discuss the NFP technology impact in applications such as single cell gene delivery, stem cell research, drug discovery, and cell cloning.

Narayana Aluru (University of Illinois at Urbana-Champaign)

TBA

SESSION 6 – 11:20 a.m., Thurs., Sept. 26

Xiaodong Li (University of Virginia) is a Rolls Royce Professor in the Department of Mechanical and Aerospace Engineering at the University of Virginia. His research interests include nanomanufacturing, nanomaterial-enabled energy systems, surface engineering, biological and bio-inspired systems and devices, biomaterials, nano/biomechanics, and mechanics and tribology in nuclear and/or turbine energy systems. He has published more than 185 peer-reviewed journal articles and his publications have been cited more than 4,000 times with an H-index of 31. He serves as associate editor for Transactions of the ASME *Applied Mechanics Reviews*, and is on the editorial board for 10 journals.

Structural Origin of Flaw Tolerance in Nacre

Nacre is a natural nanocomposite with superior mechanical strength and eminent toughness. What is the secret recipe that Mother Nature uses to fabricate nacre? What roles do the multiscale structures play in the strengthening and toughening of nacre? Can we learn from this to produce nacre-inspired nanocomposites? The recent discovery of nanoparticles in nacre is summarized, and the roles these nanoparticles play in nacre's strength and toughness are elucidated. Rotation and deformation of aragonite nanoparticles are the two prominent mechanisms contributing to energy dissipation in nacre. The biopolymer spacing between nanoparticles facilitates the particle rotation process. Individual aragonite nanoparticles

are deformable. The advancing crack invades the aragonite platelet and, simultaneously, leaves a zigzag propagation path. Dislocation formation and deformation twinning were found to play important roles in the plastic deformation of individual nanoparticles, contributing remarkably to the strength and toughness of nacre upon dynamic loading.

Nikhil Koratkar (Rensselaer Polytechnic Institute) is the John A. Clark and Edward T. Crossan Professor of Engineering at the Rensselaer Polytechnic Institute. He holds joint appointments in the Departments of Mechanical, Aerospace, and Nuclear Engineering, and Materials Science and Engineering at Rensselaer. Koratkar's research work has focused on the synthesis, characterization, and application of nanoscale material systems. This includes graphene, graphene oxide, carbon nanotubes, and fullerenes, as well as metal and silicon nanostructures produced by a variety of techniques such as exfoliation of graphite, chemical vapor deposition, and oblique angle sputter and e-beam deposition. Additional information regarding Koratkar's research can be accessed at his homepage: rpi.edu/~koratn.

Wetting Translucency of Graphene

In my talk, I will show that a monolayer graphene coating does not significantly disrupt the intrinsic wetting behavior of surfaces, where the substrate-water interaction is dictated by Van der Waals (i.e., non-bonding) forces and the underlying substrate is significantly more wettable than graphene. For such surfaces, the graphene remains transparent to the substrate wetting behavior and remains noninvasive to the substrate-water interface. We call this effect the wetting transparency of graphene. Increase in the number of graphene layers results in the contact angle transitioning gradually toward the bulk graphite value and with more than six layers resulting in the water contact angle identical to that of bulk graphite. Molecular dynamics simulations and continuum predictions (using the effective interface potential) indicate that graphene's wetting transparency is related to its extreme thinness, which only slightly perturbs the Van der Waals interaction of water to the underlying substrate.

The wetting transparency of graphene is, however, lost on super-hydrophilic surfaces where the wettability is dominated by short-range chemical bonding such as the hydrogen bonding networks that are typical of the water-glass interface. The wetting transparency effect is also lost on super-hydrophobic surfaces, which are less wettable than graphene. I will also show how minimally invasive (i.e., ultra-sheer) graphene drapes can be used to minimize droplet pinning and contact angle hysteresis on nano-patterned (i.e., rough) surfaces leading to enhanced droplet mobility, which is required for a number of applications in micro- and nano-fluidics.

SESSION 7 – 2 p.m., Thurs., Sept. 26

Jean-Pierre Leburton (University of Illinois at Urbana-Champaign) is the G. Stillman Professor of Electrical and Computer Engineering and professor of physics at the University of Illinois in Urbana-Champaign. He is also a full-time faculty member at the Beckman Institute. He received his license (B.S.) and Ph.D. in solid state physics from the University of Liege, Belgium, in 1978. Dr. Leburton joined the University of Illinois in 1981 from Germany, where he worked as a research scientist with the Siemens A.G. Research Laboratory in Munich. He is involved with research in nanostructures modeling and in quantum device simulation. His present research interest encompasses non-linear transport in quantum wires, carbon nanotubes, graphene, and molecular and ionic transport through semiconducting nanopores for biomolecule manipulation and sensing.

Multi-Function Semiconductor Membranes with Nanopore for Bio-Molecule Sensing and Manipulation

In the recent years there has been a tremendous interest in using solid-state membranes with nanopores as a new tool for DNA and RNA characterization and possible sequencing. Among solid-state nanoporous membranes the use of mono-layer graphene is particularly attractive because of its electric versatility, physical robustness, and good electronic properties. In this talk I will review progresses made with semiconducting membranes for manipulating and sensing bio-molecules. In this context, I will present a scenario that integrates biology with graphene-based nano-electronics for probing the electrical activity of DNA molecules during their translocation through a graphene membrane nanopore, thereby providing a means to manipulate them, and possibly identify electronically their molecular sequences.

Wanliang Shan (Carnegie Mellon University)

Bioinspired Design of Wearable Device with Electrically Tunable Rigidity

Laminate composites of elastomer and low melting point alloy have been demonstrated to be capable of reversible rigidity change by up to four orders of magnitude. The challenging issue remains as how to design reliable structures and devices to capitalize on such a dramatic change. In this study, we turn to nature to seek insights on potential designs toward wearable devices with tunable rigidity. The effects of various design factors and parameters are simulated using FEM and a prototype device is fabricated based on the modeling results.

Yulia Maximenko (University of Illinois at Urbana-Champaign)

Microcapsules for Luminescent Tracking and Controlled Drug Delivery

Polyelectrolyte microcapsules are formed on porous calcium carbonate templates that are impregnated and coated with 2.9 nanometer luminescent silicon nanoparticles. The complexes are characterized in suspension as well as in thin films using fluorescence microscopy, optical microscopy, and x-ray photospectroscopy. The calcium carbonate templates are thereafter dissolved by incubation of the complexes in hydrochloric acid. Polymer layer after dissolution stays intact retaining the fraction of nanoparticles inside. Simultaneous impregnation of drug biomacromolecules and Si nanoparticles may enable sensitive optical tracking of drug delivery along with the controlled drug release upon breaking a capsule with laser irradiation or ultrasound. Impregnation of the calcium carbonate microparticles with magnetic Er-Si nanoparticle complexes may in turn enable ways for magnetic interrogation.

SESSION 8 – 3:50 p.m., Thurs., Sept. 26

Wayne Chen (Purdue University) received his Ph.D. in Aeronautics at Caltech in 1995. He is currently a professor of aeronautics, astronautics, and materials engineering at Purdue University. His research interests are in dynamic experimental technique development and dynamic material characterization. His precision dynamic experimental methods have been transferred to numerous laboratories. He is a Fellow of ASME and SEM, and an Associate Fellow of AIAA.

Dynamic Mechanical Responses of Soft Biological Tissues

Mechanical responses of soft tissues at the strain rates beyond 50/s are not well documented and understood. Part of the reason for the scarcity of valid data is the lack of reliable experimental techniques to obtain such data. At these strain rates, hydraulic machines typically must operate in open-loop mode with less control on testing conditions. Split Hopkinson or Kolsky bars need modifications to obtain valid results. In a Kolsky bar experiment, specimen response itself significantly affects the testing conditions. During any test for material properties, the specimen should deform uniformly under an equilibrated stress state, such that the response averaging over the specimen volume may serve as an accurate representative of point-wise valid material properties. These testing conditions are not satisfied automatically in a Kolsky bar experiment, especially when the sample material is soft and strain rate is high. To obtain valid dynamic experimental results, modifications specifically designed for soft material testing must be introduced. This presentation introduces the challenges associated with the Kolsky bar experiments on soft tissues and presents remedies to obtain valid dynamic properties for skin, muscle, kidney, and brain tissues.

Elizabeth Horstman (University of Illinois at Urbana-Champaign)

A Microfluidic Approach for Cocrystallization of Drugs and Analysis via X-Ray Diffraction

The process of pharmaceutical drug development is cost- and time-intensive. Candidate drugs (CDs) are screened with many counter ions (salt or cocrystal formers) to find solid forms of the drug with appropriate physicochemical (e.g., solubility, dissolution rate) properties. Cocrystals are multicomponent assemblies, such as CD and counter ion, which are held together with non-covalent interactions (typically hydrogen bonding). Cocrystallization is a convenient way to alter the physical properties of a solid form without affecting the chemical identity of the CD.

Cocrystals can be generated via methods including solvent-assisted grinding, temperature control, antisolvent addition, and solvent evaporation. A crystal structure of the resulting cocrystal is often desired. However, growing good quality cocrystals that can be analysed using single crystal x-ray analysis is challenging.

My research objective is to develop an integrated microscale total analysis system to enhance cocrystallization by utilizing an on-chip seeding approach followed by on-chip analysis of solid forms via Raman spectroscopy and x-ray diffraction. The specific aims of my research are: (1) design and fabricate a solvent compatible and x-ray transparent multiplexed microfluidic platform (72 individually addressable, 100 nl wells) for cocrystal seeding to grow diffraction quality crystals; (2) employ Raman spectroscopy and x-ray diffraction to identify cocrystals on-chip.

The microfluidic platform is comprised of thin poly (dimethylsiloxane) fluid and control layers. These layers are sandwiched between cyclic olefin copolymer substrates that are solvent impermeable thereby minimizing solvent loss during crystallization. The control layers have normally closed valves that are used for fluid routing and mixing. The microfluidic platform allows for portability between the solution loading and the analysis stations. To conduct Raman and x-ray analysis on-chip, the device materials need to be Raman and x-ray transparent in order to minimize background noise. Cyclic olefin copolymer is Raman and x-ray transparent and the poly (dimethylsiloxane) layers were minimized to decrease x-ray absorption. This platform was designed to be less than 200 um thick. To circumvent the need to harvest the crystals for downstream analyses and the need to grow large isolated x-ray quality crystals, I intend to grow many, small crystals on-chip via seeding approach and collect small wedges of x-ray data. The many small crystals on the platform are assumed to be randomly oriented. By taking small wedges of data from many crystals a complete crystal structure can be solved.

Harvesting crystals from the microfluidic platform is a tedious process that may damage the crystals and compromise the x-ray data and therefore is avoided. On-chip analysis allows for x-ray data to be collected at room temperature which provides more accurate lattice parameters as opposed to cryocooling of single crystals during traditional x-ray analysis.

Zhao Qin (MIT)

Multi-Scale Modeling of Protein Materials and Their Mechanics

Nature provides a very rich database of biological materials such as spider silk, nacre, and cytoskeleton. These materials have fascinating structures and outstanding mechanical functions by assembling at very low energy cost. They are composed of simple basic material building blocks, defined by the chemical structures of the molecules. Here we present a coupled computational-experimental approach applied to investigate the interplay between architectures and mechanics of protein materials at multiple scales, and exploit the knowledge to design and synthesize novel protein materials. We explain how hierarchical structure from single molecules to macroscopic level provides a route to achieve great strength and flexibility in design. Each level serves as a building block and contributes to the overall properties, but the remarkable function of the material emerges because of the synergistic organization across different scales, making the whole more than the collection of its parts. By translating this insight gained from the study of natural materials such as mussel glue, spider silk, or intermediate filament to engineered materials such as carbon nanotube fibers or graphene composites, we demonstrate an engineering paradigm that facilitates the design of sustainable and multi-functional materials starting from the molecular level.

Friday's Speakers:

CHAITANYA SATHE 9 a.m.

An Introduction to Computational Modeling using VMD and NAMD

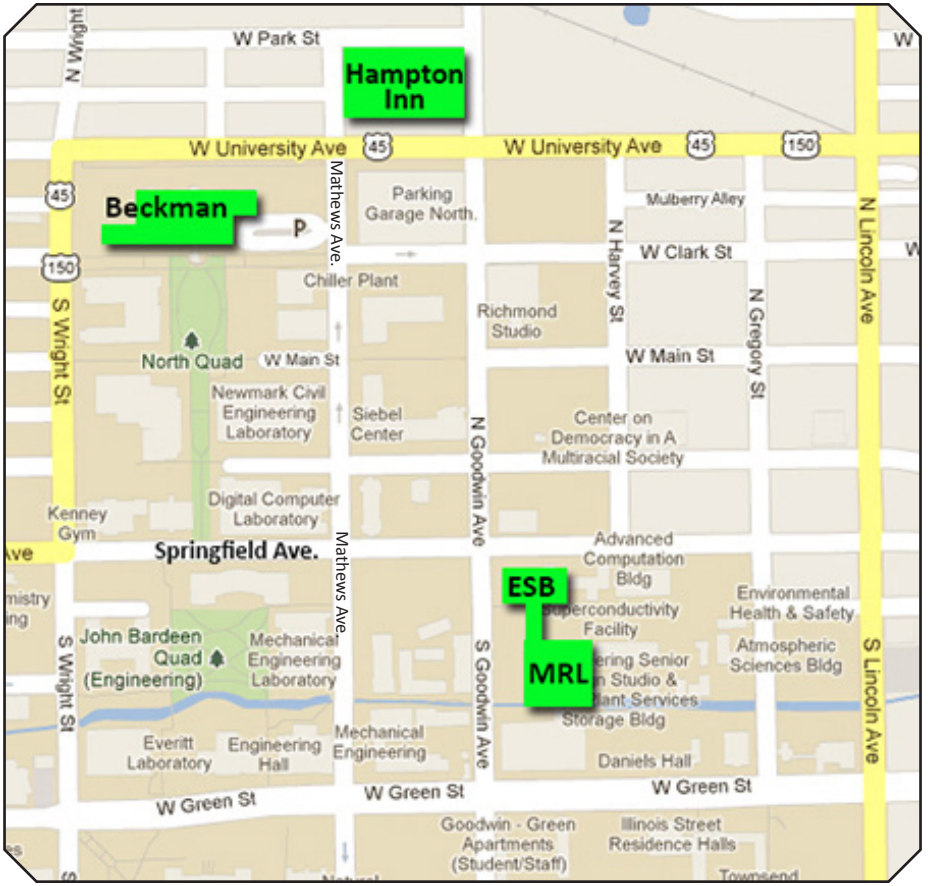
MAXIM BELKIN 11 a.m.

Overview of Advanced NAMD Features and Their Application in Simulations

Map of the 2nd floor of the MRL

You will need your lunch tickets (inside your name tag holder) to pick up lunch in Room 201 MRL.

Map for the MRL, Beckman, and Hampton Inn



Materials Research Laboratory
104 South Goodwin Ave.
Urbana, IL 61801

mrl.illinois.edu

Beckman Institute
405 North Mathews Ave.
Urbana, IL 61801

beckman.illinois.edu