

Materials Science and Engineering

**Erik Luijten**

Associate Professor
Materials Science and Engineering
and
Engineering Sciences and Applied Mathematics
Northwestern University

Tuesday, October 8, 2013
Tech L211, 4:00pm

Self-Assembly: From Algorithms to Gene Delivery

Erik Luijten will give a broadly accessible overview of recent findings in his group in the field of self-assembly. He will highlight novel mechanisms controlling out-of-equilibrium self-assembly, the design of nanoparticles for gene therapy, algorithmic advances that have made it possible to explore new phenomena in colloidal suspensions, and even new insights into the surface organization of bacteria.

1. J. Yan *et al.*, *Nature* **491**, 578–581 (2012).
2. D.W. Sinkovits and E. Luijten, *Nano Lett.* **12**, 1743–1748 (2012).
3. X. Jiang *et al.*, *Adv. Mater.* **25**, 227–232 (2013).
4. K. Zhao *et al.*, *Nature* **497**, 388–391 (2013).

Biography: Erik Luijten holds degrees in Theoretical Physics from Utrecht University and Delft University of Technology.

He specializes in the study of soft condensed-matter systems by means of large-scale computer simulations. These materials, also known as complex fluids, comprise colloidal suspensions, polyelectrolytic systems, ionic solutions, and other nanoscale systems in the liquid state. Their intrinsic complexity necessitates the development of advanced simulation algorithms and analysis tools. Erik Luijten has contributed several Monte Carlo methods that are now considered the state of the art in their fields of application, including algorithms that greatly accelerate calculations for multicomponent fluids and for systems with long-range interactions. His current research concentrates on the development of biomaterials for gene delivery, the self-assembly of viruses and synthetic anisotropic building blocks, and the role of electrostatic and dielectric effects in the phase behavior of fluids.

Erik Luijten received an NSF CAREER Award, a Xerox Award for faculty research, and the Helmholtz Award for fundamental and innovative contributions enhancing the state of the art of computer simulations of aqueous solutions.

Dr. Timothy Fister

Assistant Staff Scientist

Chemical Sciences and Engineering Division
Argonne National Laboratory**Tuesday, October 15, 2013****Tech L211, 4:00pm****“Interfacial Control of Lithiation Using Layered Intermetallic Architectures”**

Next generation lithium battery materials will require a fundamental shift from intercalation materials to elements or compounds that alloy directly with lithium. Intercalation compounds, like graphite and $LiCoO_2$, provide a stable crystal structure with open sites for mobile lithium ions, but are intrinsically limited in their energy density by the weight and volume of the host material. Intermetallics can electrochemically alloy to $Li_{4.4}M$ ($M = Si, Ge, Sn, \text{etc}$), providing order-of-magnitude increases in energy density. However, this process leads to volume changes (up to 300%) that rapidly degrade the performance of the battery due to delamination between the active material and its underlying current collector. Using *in situ* x-ray reflectivity, we have studied a model interface using a bilayer of silicon and chromium that act as an anode material and current

collector respectively. We find that the interface is intermixed, but stratifies into distinct $CrSi_x$ layers; during lithiation, these layers vertically phase-separate into alternating $LiSi_x$ phases and more chromium-rich $CrSi_x$. Drawing from the structural stability of the layered silicides, we have recently grown larger-scale silicon/chromium multilayers, e.g. repeating the bilayer structure 20-50 times. With higher silicon content, these multilayers reversibly show 3.3-fold expansion and contraction while still maintaining their layered structure, as seen by *in operando* x-ray reflectivity. The electrodes also give substantial improvement over pure-phase silicon thin films in both long-term cycling and high power applications. Multilayers using Ge and Ti also provide similar reversibility and performance. Constraining the alloying reaction in such a layered architecture appears to lead to structural behavior similar to more traditional intercalation compounds and may be useful for higher voltage alloying reactions in metal oxides and sulfides.

Biography: Tim Fister received his B.S. at the University of Minnesota and his Ph.D. in physics at the University of Washington before arriving at Argonne. His research centers on the development of synchrotron-based x-ray techniques to understand the structural and electronic properties of materials for energy conversion and storage at working conditions.

Materials Science and Engineering

**Monika Backhaus-Ricoult**
Corning Incorporated**Tuesday, October 22, 2013**
Tech L211, 4:00pm**Exchange Processes at Oxide Electrode Surfaces for SOFC, Sensor and Electrochemical Reactor Applications**

Electrode transport and exchange processes play a critical role for the performance of solid oxide fuel cells, gas sensors, gas separation membranes and electrochemical reactors. They depend on bulk, surface and interface chemistry and are affected by changes in chemical composition, stoichiometry and structure during processing and/or high temperature device operation. Studies of the surface chemistry of oxide catalysts and associated reaction mechanisms under different operation conditions are needed to gain a broader understanding of the catalysts and their activity and help to assess and overcome performance limitations of electrochemical devices.

As part of exploratory research on energy-related devices at Corning, we studied oxygen reduction in SOFC cathodes, NO_x reduction in model sensors and hydrocarbon oxidation processes at mixed oxide and metal electrodes. We used a combination of impedance spectroscopy, electrochemical relaxation response analysis, bulk and surface diffusion experiments, microscopy and surface spectroscopy to gain information on the various parallel and sequential reaction steps contributing to oxygen reduction reaction and oxygen excorporation. We developed a spatially resolved in-situ scanning photoelectron microscopy approach to study the response of electrode surfaces at a macro- and micro-scale to changes in temperature, oxygen (NO_x, hydrocarbon) gas pressure and polarization during high temperature operation of electrochemical model cells. Results of those experiments will be presented.

Biography: Dr. Monika Backhaus-Ricoult is currently Senior Research Associate in Crystalline Materials Research at Corning Incorporated in Corning, New York. She was trained as a physical chemist and earned her Ph.D. in Physical Chemistry at the University of Hannover, Germany.

Monika joined Corning in 2003 after 18 years of academic research experience, as Research Director at the National Research Center (CNRS) in Paris, France, Adjunct Professor at Cornell University, Research Scientist at the Max Planck Institute (Stuttgart, Germany) and Research Assistant at the University of Hannover. During these years, Monika conducted and guided research and had several teaching appointments. Research activities included solid state reactivity, transport and morphology evolution, high temperature corrosion, high temperature plastic deformation, interface structure and chemistry at atomistic scale. Monika's key area of interest was and remains the reactivity and electrochemistry of interfaces

She holds 29 patent applications and is credited with 130 publications, as well as 88 Corning internal technical reports. Since joining Corning, Monika is recognized as an expert of ceramic properties, microstructure and processing. She has worked on porous ceramics for diesel particulate filter applications, SOFC, electrochemical sensors, thermoelectrics and is engaged in material research for energy applications. Her "research hobbies" include in-situ studies of interfacial and surface phenomena by electron microscopy and spectroscopy.



Dr. Milan K. Sanyal

Director and Senior Professor
Saha Institute of Nuclear Physics
Kolkata, India

Tuesday, October 29, 2013
Tech L211, 4:00pm

“Nano-crystal Formation at Interfaces”

Fascinating physical properties evolve in materials when it gets confined in any of the three physical directions. We shall first discuss here the results of a study to understand the formation mechanism of single crystals of the transition metal chalcogenide, CuS, at the water–toluene interface through an interfacial reaction. Systematic measurements carried out using synchrotron x-ray scattering (at ESRF), electron microscopy, atomic force microscopy and calorimetric techniques clearly show that nano-crystallites of CuS form within a few minutes at the interface as the reagents are brought from the organic (upper) and aqueous (lower) layers to the interface, then crystallization of CuS proceeds over a few hours only by reorganization, despite the large excess available in both upper and lower liquid phases. The interface confinement and passivation by organics is critical here in the formation of single crystals having sizes of 6 and 200 nm along the normal and in-plane directions of the liquid–liquid interface.

In Si/Ge heteroepitaxy, alloying plays an important role in strain-relaxation in formation Ge-dots at the buried interfaces. Following recent development in this field, we could grow in lower temperature deposition the inverse quantum hut structure that grows within silicon layer. The enigmatic diffusion of Ge in the lower Si-sub-layer at lower temperature (<400°C) and formation of “inverse hut” structure is not yet understood. We have carried out a study of MBE grown Si/Ge superlattice structures using Cross-sectional transmission electron microscopy (XTEM) and anomalous grazing incidence diffraction (GID) techniques. Anomalous X-ray scattering measurements refer to setting the energy of X-ray close to the absorption edge of a particular material to increase the sensitivity of X-ray for that material. The results of these XRD studies at Ge-edge carried out at PETRA-III, DESY will be presented here.

Biography: Milan K. Sanyal is the Director and senior Professor at Saha Institute of Nuclear Physics (SINP) – an autonomous institute in the Department of Atomic Energy – in Kolkata, India. He joined SINP in 1995 to initiate a research group in surface physics. Before joining SINP, he was a Scientific Officer in Bhabha Atomic Research Centre, Mumbai from 1977 and was a Research Associate in Brookhaven National Laboratory, USA from 1989 to 1992. Prof. Sanyal is a fellow of all three academies of sciences in India, namely Indian National Science Academy, Indian Academy Sciences and The National Academy of Sciences, India. He is a member of several important national committees, like the Science Advisory Committee of the Cabinet, Government of India (SAC-C), India-Japan Science Council and Nano-Science committee of India. Prof. Sanyal’s research interests are synchrotron x-ray and neutron scattering studies of surface and interfaces, structure-property correlation in low-dimensional systems and electronic transport properties in nano-structured materials.



Professor Ram Seshadri

Materials Department & Department of Chemistry and Biochemistry
Co-Director, Materials Research Laboratory
University of California – Santa Barbara

Tuesday, November 5, 2013
Tech L211, 4:00pm

“Solid-state Chemistry in Energy Efficiency: Lighting Phosphors and Thermoelectric Materials”

In the first part, I will address phosphors that play a key role in the now almost-mature solid-state white-lighting technologies based on combining a III-nitride-based near-UV or blue solid-state light source with down-conversion to longer wavelengths.[1] Almost all widely used phosphors comprise a crystalline oxide, nitride, or oxynitride host that is appropriately doped with either Ce^{3+} or Eu^{2+} . Optical excitation into these states and concomitant reemission can be tuned into the appropriate regions of the visible spectrum by the crystal these ions are hosted in. Experimental studies of some of the best phosphor materials, employing state-of-the-art structural tools, have yielded guidelines for what are desirable structural features. We find that a useful sorting diagram for efficient hosts with high quantum yield has the band gap of the host – readily calculated with high reliability using hybrid functionals in DFT – as one of the axes, and the calculated Debye temperature as the other axis.[2]

In the second part, I will describe the creation of a large database of thermoelectric materials prepared by abstracting information from over 100 publications. Appropriate visualization of the data immediately allows certain insights to be gained with regard to the property space of plausible thermoelectric materials. The Herfindahl–Hirschman index – a commonly accepted measure of market concentration and monopoly – has been calculated from geological data (known elemental reserves) and geopolitical data (elemental production) for much of the periodic table. The visualization strategy employed allows rapid sorting of thermoelectric compositions with respect to important issues of elemental scarcity and supply risk.[3]

- [1] N. C. George, K. A. Denault, and R. Seshadri, Phosphors for solid-state white lighting, *Annu. Rev. Mater. Res.* **43** (2013) 481–501.
- [2] J. Brgoch, S. P. DenBaars, and R. Seshadri, Proxies from *ab-initio* calculations for screening efficient Ce^{3+} phosphor hosts, *J. Phys. Chem. C (online)*.
- [3] M. W. Gaultois, T. D. Sparks, C. K. H. Borg, R. Seshadri, W. D. Bonificio, and D. R. Clarke, A data-driven review of thermoelectric materials: Performance and resource considerations, *Chem. Mater.* **25** (2013) 2911–2920.

Biography: Ram Seshadri has been on the faculty of the University of California, Santa Barbara since 2002, where he is currently Professor of Materials and Professor in the Department of Chemistry and Biochemistry, in addition to co-Directing the Materials Research Laboratory, the NSF MRSEC at UCSB. Research carried out in his group combines aspects of physics, chemistry, and materials science, within the broad theme of crystal chemistry, and crystal-structure–property relations in functional inorganic materials. Functions of current interest include solid-state lighting, magnetism, thermoelectricity, and energy storage.

Materials Science and Engineering

**Izabela Szlufarska**

Associate Professor,
Materials Science and Engineering Department
University of Wisconsin-Madison

Tuesday, November 12, 2013
Tech L211, 4:00pm

**Toward Computational Design of Wear Resistant Materials:
Molecular Understanding of Friction**

It has been estimated that about one third of energy produced in industrialized countries is lost to overcoming friction. Significant reduction in this loss can be made through design of coating materials with superior tribological properties for use in transportation and industrial production. Although knowledge of fundamental mechanisms underlying friction can enable rational and systematic design of coatings, such an approach has been hindered by the limited understanding of basic physical and chemical processes taking place in the sliding contact. The basic laws of friction were first proposed by Leonardo da Vinci in 1699. However, even centuries after this discovery it is still not possible to quantitatively predict friction parameters, such as friction coefficient and interfacial shear strength. The challenges in understanding friction stem from the complexity of energy dissipation mechanisms involved in sliding, which include elastic instabilities, phonon and electronic dissipation, dislocation motion, chemical reactions at the interface, and others.

A transformation of the field of tribology has been recently enabled by the convergence of length scales accessible to experimental studies and to fully atomistic simulations of contact mechanics. In this talk I will discuss specific examples of insights into nanoscale tribology gained from my work using large-scale molecular dynamics simulations with highly realistic empirical potentials combined with *ab initio* modeling. One example is the discovery of mechanisms that underlie aging of silica in aqueous environments, which is of interest for multiple phenomena ranging from wafer bonding to shallow tectonic earthquakes. My group has demonstrated that in the absence of deformation creep, aging of silica takes place by formation of interfacial siloxane bridges. We have discovered a new mechanism for interaction between these bridges and have shown that this interaction is critical to explain experimentally observed logarithmic dependence of aging on time. I will also discuss contributions from my group to understanding of deformation and wear of nanocrystalline materials. For instance, we discovered deformation mechanisms in ultrananocrystalline diamond and explained the effects of H dopants on mechanical properties of this material. We have shown that in the absence of dislocation plasticity, yield stress and hardness of nanocrystalline materials scale with grain boundary shear strength. Finally, I will discuss our recent developments of theories and algorithms that enable bridging of time scales between molecular simulations and experiments, with a particular focus on friction and slip at solid/liquid interfaces

Biography: Izabela Szlufarska is an associate professor in the Department of Materials Science & Engineering at the University of Wisconsin (UW) – Madison. She also holds an affiliate appointment in the Department of Engineering Physics. Szlufarska joined UW-Madison in 2004 as an assistant professor and was promoted to an associate professor with tenure in 2010. In 2011 she spent a yearlong sabbatical at MIT as a visiting associate professor in the Department of Materials Science & Engineering. At UW-Madison Szlufarska co-leads the Computational Materials Group, which at present has over 30 members. She is also the founder and the leader of the Interdisciplinary Computational Group (ICG), which is a virtual group within the UW Materials Research Science and Engineering Center (MRSEC) that brings together researchers from five different departments across the UW campus. Szlufarska's research falls into two general areas: nanomechanics and materials for nuclear energy applications. Within nanomechanics, Szlufarska develops and uses multi-scale simulation approaches to study adhesion, friction, and wear in solid/solid and solid/liquid contacts. She received a number of professional awards, including NSF CAREER award and AFOSR Young Investigator Program Award.

Materials Science and Engineering

**Dr. Eric Stach**

Brookhaven National Laboratory
&
Hummingbird Scientific

**Tuesday, November 26, 2013
Tech L211, 4:00pm**

Environmental Transmission Microscopy for Catalysis Research: The Example of Carbon Nanotubes

Crucial to the application of Nano structured materials is control over their nucleation and growth, as these aspects determine their structure and thus properties. I will describe how we can exploit the unique capabilities of in situ environmental cell transmission electron microscopy (ETEM) to observe multiple aspects of these processes. With this approach we can directly visualize how the catalysts that mediate nanotube growth respond to various changes in the growth environment and correlate these changes with the resulting nanotubes structures.

In the first portion of the presentation we will investigate how dynamic changes in catalyst morphology are correlated with the termination of growth in vertically aligned single-walled nanotube arrays. In particular, we have investigated how nanotubes nucleate and self-organize into vertical arrays, as well as the processes of catalyst coarsening, Ostwald ripening and diffusion into the catalyst support that lead to growth termination. In particular, I will describe how changes in the growth feedstock - in particular the incorporation of controlled amounts of water vapor - can alter the catalyst evolution.

In the second portion of the presentation, I will describe how altering other aspects of the growth feedstock - in this case the carrier gas, in combination with the water vapor content - can affect not only the catalyst morphological evolution but can also significantly bias the chiral distribution of the resulting nanotubes. Changes in the growth ambient are correlated with a roughening transition, which leads to a change in the rate of Ostwald ripening.

Finally, ongoing developments of the ETEM technique will be presented, focusing on control of gas streams, improvements in data acquisition and correlative studies with x-ray absorption spectroscopy. Extension of the observations of morphological changes in carbon nanotube growth to broader studies in catalysis will be outlined.

Biography: Eric Stach leads the Electron Microscopy Group in the Center for Functional Nanomaterials (CFN) at Brookhaven National Laboratory. He received his Ph.D. in Materials Science and Engineering from the University of Virginia. He has held positions as Staff Scientist and Principal Investigator at the National Center for Electron Microscopy at the Lawrence Berkeley National Laboratory and as Associate then Full Professor at Purdue University, where he retains an Adjunct appointment. He is also Co-founder and CTO of Hummingbird Scientific, a nanotechnology company focusing on advanced characterization equipment.

His research interests focus on the development and application of electron microscopy techniques to solve materials problems in nanostructure growth, catalysis, thin film growth and materials deformation. Dr. Stach is a Fellow of the Microscopy Society of America, and has received several awards, among them the Microscopy Society of America's Eli F. Burton (Young Scientist) Award, and Purdue University's Faculty Scholar and Early Career Research Excellence Awards. He is the author of over 200 peer-reviewed publications, and has given over 150 invited presentations at conferences and university, corporate and national laboratories.

Materials Science and Engineering

**Dr. Michael Norman**

Director, Materials Science Division
Distinguished Fellow
Argonne National Laboratory

Tuesday, January 14, 2014
Tech L211, 4:00pm

“Materials Design for Superconductors”

Recently, there has been a lot of hoopla over the Materials Genome Initiative and how this might accelerate materials discovery. But predicting new ferroelectrics or battery materials is one thing, predicting new superconductors is quite the different matter. In fact, there have been a number of attempts to do this going back many decades with somewhat limited success. In this talk, I would like to survey recent attempts to apply Materials Genome and related ideas in the quest for new superconductors, discussing the failures, but also the successes, and what the future might have in store for us.

Biography: Mike Norman is Argonne Distinguished Fellow and Director of the Materials Science Division at Argonne National Laboratory. He is also a PI in the Center for Emergent Superconductivity, a DOE Energy Frontier Research Center. Mike became a Fellow of the American Physical Society in 1995, received the University of Chicago Distinguished Performance Award in 1999, and was on the Editorial Board of Physical Review B from 2000-2005.

Mike got his PhD in Physics in 1983 at Tulane University. After a postdoc on electronic structure at Argonne and Northwestern University, he turned to many body theory, working primarily on heavy fermion and high temperature cuprate superconductors. His other interests include spin liquids, quantum criticality, and the interpretation of spectroscopic data. He is an author on over 200 publications.

Materials Science and Engineering

Philipp Heck

Robert A. Pritzker Associate Curator of Meteoritics and Polar Studies
Field Museum of Natural History

Tuesday, February 04, 2014
Tech L211, 4:00pm

Cosmochemistry meets Materials Science



Cosmochemistry is the science of the study of extraterrestrial materials in the laboratory. Objects of study range from meteorites and their components, extraterrestrial dust collected in sediments, ice and the atmosphere to extraterrestrial samples returned to Earth by space missions. The study of the physical properties, the mineralogical and chemical compositions of extraterrestrial materials helps to understand origin and evolution of our solar system. Techniques that have been developed for materials science have become essential in cosmochemistry. Established techniques used in cosmochemistry include electron microscopy, and secondary ion mass spectrometry, more novel techniques in the field include focused ion beam microscopy, X-ray computed tomography and atom-probe tomography. I will give examples from my own research how the application of such techniques will help to better understand the history of the solar system.

Biography: Philipp R. Heck is the Robert A. Pritzker Associate Curator of Meteoritics and Polar Studies at the Field Museum of Natural History in Chicago, IL. He is also a member of the Chicago Center for Cosmochemistry at the University of Chicago. Heck directs the research program in meteoritics at the Field Museum and oversees the collection of meteorites; the largest meteorite collection housed at a private institution. Other responsibilities include the curation of the gem, mineral, rock and economic geology collections. Heck is a member of the international research consortium to study the first modern interstellar dust returned by NASA's Stardust Mission. He obtained his M.Sc. and Ph.D. degrees at ETH Zurich in Switzerland in geo- and cosmochemistry and was a postdoc at the Max-Planck-Institute for Chemistry in Mainz, the University of Wisconsin-Madison and the University of Chicago.



Prof. Seth Fraden

Professor of Physics
Brandeis University

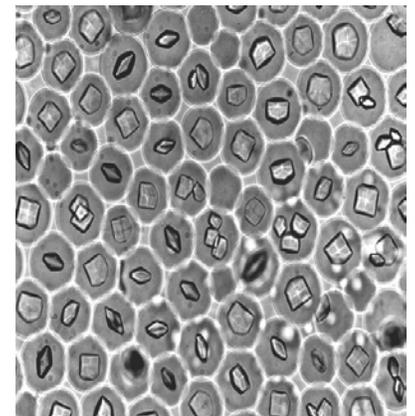
Tuesday, February 11, 2014
Tech L211, 4:00pm

“Microfluidics for Protein Crystallization”

Transformation of a protein solution to a crystal is governed by two non-equilibrium processes; nucleation and growth. Consequently, supersaturation kinetics plays an essential role in crystallization and we argue that the optimal crystallization strategy should screen kinetic trajectories involving non-thermodynamic variables such as depth of supersaturation, duration of supersaturation, and sample volume.

We have developed a technology based on emulsion microfluidics in which 1 nl drops of protein solution are encapsulated in oil and stabilized by surfactant. Crystallization is a stochastic process; we determine nucleation kinetics by measuring thousands of identical drops. We optimize nucleation and growth by generating hundreds of different kinetic paths simultaneously by varying both temperature and concentration of the protein solution.

Our objective is to produce microfluidic devices ideal for in situ structure studies by synchrotron diffraction. This entails finding conditions on chip for which one crystal is grown per drop and then isolating hundreds of drops stored on a x-ray transparent microfluidic chip. Single, non-cryoprotected crystals are too small to collect a complete diffraction data, but a full data set can be obtained by combining many single diffraction patterns. Proof of principle experiments will be presented.



Biography: Professor Seth Fraden received his undergraduate B.A. in Physics from the University of California, Berkeley, U.S.A. in 1979 and his PhD in Physics from Brandeis University, Massachusetts, U.S.A. in 1987. He worked as an NSF postdoctoral Fellow from 1987 – 1989 at the Max Planck Institute Hochfeld Magnetlabor in Grenoble, France. In 1989 he joined the physics department at Brandeis University. Seth’s research is in the area of soft condensed matter, non-linear chemical dynamics, protein crystallization, microfluidics and biomaterials and is director of the NSF Materials Research Science and Training Center (MRSEC) at Brandeis University. Website: <http://fraden.brandeis.edu/>

Materials Science and Engineering



Dr. Roland Pellenq
Senior Research Scientist
Massachusetts Institute of Technology

Tuesday, February 25, 2014
Tech L211, 4:00pm

Transport Properties of Alkanes in Shale-Rocks from the Bottom-Up Approach

Oil and natural gas from deep shale formations are expected to greatly impact the entire world economy as these are spread out everywhere around the globe. The abundance of shale gas resources worldwide—and the fact that burning natural gas emits less CO₂ than other fossil fuels—has created the expectation of a golden age of natural gas in a global energy system. This revolution relies on the large-scale deployment of new technologies allowing the production of hydrocarbons (oil, and especially natural gas), from source rock formations that were considered unproductive until very recently. The modeling of the hydrocarbons flow in nanoporous rocks such as shale has become an important new area of fluid mechanics. Gas/oil shale are sedimentary rocks with ultralow permeability. Estimates of long-term production and technically recoverable resources are, however, highly uncertain. The fundamental mechanisms controlling shale gas extraction remain poorly understood, and the classic theories and simulation techniques used by the oil and gas industry have proven inadequate for shale source rocks. Flow through shale poses a distinctive challenge that is new to the oil and gas industry: a large part of pores in shale have typical widths in the order of a few angstroms, and are within an organic porous material (kerogen) containing adsorbed hydrocarbons. At these scales, the pore size is on the order of the mean free path of the hydrocarbon molecules, and the Navier–Stokes equations with no-slip boundary condition cannot adequately represent the flow.

In the present talk, a generic model describing the flow in a multi-scale porous medium (such as shale) and fully taking into account the thermodynamics of confined fluids in nano and sub-nanopores, (including adsorption processes) is proposed without postulating any transport or diffusion mechanism. The model assumes that the rock pore void consist of different types of domains with different of pore sizes starting at the sub-nanometer level with a realistic atomistic description of the kerogen porosity (close to that of common porous carbons). This is a key improvement compared to current attempts to model flow (and production) in shale which all assume in the first place that the flow has to comply to Darcy's behavior. Furthermore, our approach provides for the first time firm theoretical grounds for Archie's law relating the in-situ flow to the porosity of the medium.

Biography: Dr. Roland Pellenq is a computational materials scientist with a strong interest in the physics and mechanics of micro- and nanoporous materials and confined fluids. He graduated in 1994 with a PhD in Chemical Physics from Imperial College, London; and is currently a First Class Research Director at CNRS, the French government research agency and a MIT Senior Research Scientist.

Dr. Pellenq's research is dedicated to the development of bottom-up simulation approaches (starting at an atomistic level of description) for a large variety of critical problems in energy and environment, ranging from hydrogen and CH₄ storage, CO₂ sequestration, shale gas to the stability of nuclear fuels and fundamentals of cement and concrete research. R. Pellenq is the author or co-author of 140 papers published in major peer reviewed scientific journals.

He was one of the co-founders and lead scientist of the Concrete Sustainability Hub, CSH@MIT, opened in 2009, an interdisciplinary research center dedicated to the reduction of the environmental footprint of the cement and concrete industry. He is also principal investigator of the MIT Xshale project focusing on gas-shale research.

He was hired as a MIT Senior Research Scientist in November 2010 and is the head of the CNRS-MIT joint laboratory "Multi-Scale Material Science for Energy and Environment" open in June 2012 and located on the MIT campus (Cambridge, US).

Materials Science and Engineering



Dr. Alexandra Boltasseva

Associate Professor, Electrical and Computer Engineering
and Birck Nanotechnology Center
Purdue University

Tuesday, April 29, 2014
Tech L211, 4:00pm

Empowering Plasmonics and Metamaterials Technology with New Material Platforms

In recent years, plasmonics and metamaterials have seen an explosion of novel ideas and designs that could provide breakthrough devices and exotic functionalities. However, transforming these concepts into practical devices requires a significant amount of effort. The constituent materials in these structures play a crucial role in realizing efficient devices. Similar to the way silicon shaped the nanoelectronics field, efforts toward finding the best set of materials for plasmonic and metamaterial devices could revolutionize the field of nanophotonics. As a potential solution, alternative plasmonic materials have recently gained significant attention. Metals, despite being essential components of plasmonic and metamaterial structures, pose many technological challenges toward the realization of practical devices—primarily due to their high optical loss, integration and fabrication limitations. Hence, searching for an alternative to metals is vital to the success of future nanophotonic devices. In this course, recent developments in the pursuit of better plasmonic materials will be outlined, and several classes of materials including transparent conducting oxides and plasmonic ceramics as potential alternatives to metals will be discussed as material platforms that provide low intrinsic loss, tunability and compatibility with standard semiconductor fabrication processes.

Biography: Alexandra Boltasseva is an Associate Professor at the School of Electrical and Computer Engineering, Purdue University, and an adjunct Associate Professor at Technical University of Denmark (DTU). She received her PhD in electrical engineering at DTU in 2004. Boltasseva specializes in nanophotonics, nanofabrication, plasmonics and metamaterials. She received the 2013 IEEE Photonics Society Young Investigator Award, 2013 Materials Research Society (MRS) Outstanding Young Investigator Award, the MIT Technology Review Top Young Innovator (TR35) award that "honors 35 innovators under 35 each year whose work promises to change the world", the Purdue College of Engineering Early Career Research Award, the Young Researcher Award in Advanced Optical Technologies from the University of Erlangen-Nuremberg, Germany, and the Young Elite-Researcher Award from the Danish Council for Independent Research. She is topical editor for Optics Letters, a member of the Board of directors for MRS, senior member of the OSA, member of the IEEE, SPIE. She has co-authored five invited book chapters and 74 research papers in refereed journals. She has an h-index of 33 (Google Scholar) with a total number of citations above 3000. Alexandra has been featured as an invited speaker at more than 70 international conferences and leading research centers.



Professor Pascal Bellon

Racheff Faculty Scholar, Material Science and Engineering
University of Illinois

Tuesday, May 6, 2014
Tech L211, 4:00pm

Plastic Deformation in Alloys: from mixing mechanisms to nanoscale self-organization

Materials are commonly subjected to plastic deformation during fabrication and shaping, and in service. Using analytical models, atomistic simulations, and experiments, our research has shown that metallic alloys subjected to severe plastic deformation display a rich phenomenology, from non-diffusive transport to self-organization at the nanoscale. We predicted in particular that for systems with easy slip transfer across interphase boundaries, the chemical mixing forced by plastic deformation should be superdiffusive. We will present recent experimental work investigating this prediction by subjecting Cu-Ag alloys to high pressure torsion. Another remarkable property of alloys under sustained plastic deformation is their tendency to self-organize, which results from the presence of simultaneous competing processes with distinct intrinsic length scales. We will show that these reactions can be used to design self-adapting materials with improved service properties. This point will be illustrated by showing that, under appropriate conditions, sliding wear can induce nanolayering just below the wear surface, greatly improving wear resistance.

Biography: Professor Bellon received an electrical engineering degree from Ecole Supérieure d'Électricité, France, in 1984 and a PhD in materials science from University Paris 6, France, in 1989. He then worked at the Physical Metallurgy Research Section (SRMP) at the CEA Center for Research at Saclay, France, until 1996. He first worked in the MatSE Department at UIUC as a post-doctoral fellow in 1993-1994, and joined the faculty at UIUC in 1996. He was promoted to Associate Professor in 2002 and Professor in 2009. He received an NSF Career Award in 1998, the Don Burnett Teaching Award in 2000, the Faculty Pierce Award in 2009, and was named a Racheff Faculty Scholar in 2012.

Materials Science and Engineering



Todd Hufnagel

Professor, Materials Science and Engineering
Department & Mechanical Engineering
Johns Hopkins University

Tuesday, May 27, 2014
Tech L211, 4:00pm

Deformation and Fracture of Metallic Glasses

Amorphous metallic alloys combine some of the advantageous mechanical properties of metals, such as high strength and (in some alloys) toughness, with the processing flexibility associated with materials capable of undergoing a glass transition into a supercooled liquid state. The disordered structure of metallic glasses implies that the mechanisms of deformation and fracture in these novel materials are different from those of conventional crystalline alloys.

In this talk we will review the mechanical behavior of metallic glasses and discuss several recent experiments that shed new light on mechanisms of elastic deformation, plastic deformation, and fracture. In the case of elastic deformation, high-energy x-ray scattering experiments and molecular dynamics simulations both indicate that an apparent length-scale dependence of the elastic strain is associated with localized non-affine atomic displacements that may be related to the operation of shear transformation zones (STZs). Stress-strain data recorded with high temporal resolution reveal that both scaling and dynamics of load drops during plastic flow are in excellent agreement with a simple mean-field model describing these events as avalanches of individual STZ operations. These avalanches are manifested as shear bands, and experiments designed to measure the heat released during shear band operations show that they can occur without significant heating. Finally, we show how high-energy x-ray scattering can be used to map the elastic strain state locally around crack tips in fracture specimens, and that a loss of fracture toughness at low temperature is associated with a reduction in the size of the plastic zone around the crack tip. We propose that the difference in behavior is associated with changes in the flow stress and elastic constants, which influence the number density of shear bands in the plastic zone and thus the strain required to initiate fracture on an individual band.

Biography: Todd Hufnagel is Professor of Materials Science and Engineering and Mechanical Engineering at Johns Hopkins University. He has received an NSF CAREER Award and an ARO Young Investigator Award. His current research emphasizes the use of x-ray scattering and imaging to study dynamic processes in materials.

He received his B.S. degree in Metallurgical Engineering from Michigan Tech, and M.S. and Ph.D. in Materials Science and Engineering from Stanford.

Materials Science and Engineering

**Yang-Tse Cheng**

Professor, Chemical and Materials Science Department
University of Kentucky

Tuesday, June 3, 2014
Tech L211, 4:00pm

Understanding coupled mechanical-chemical degradation mechanisms for improving the performance and durability of lithium ion batteries

Advanced lithium ion battery electrodes experience large volume changes caused by concentration changes within the host particles during charging and discharging. Electrode failure, in the form of fracture or decrepitation, can occur as a result of repeated volume changes. In this presentation, we will provide an overview of our recent work on understanding the evolution of concentration, stress, and strain energy within a spherically- or cylindrically-shaped electrode element under various charging-discharging conditions. We show that a dimensionless parameter, the electrochemical Biot number, may be used to characterize stress and strain energy evolution in an electrode. In particular, the electrochemical Biot number determines the maximum stress and strain energy. Based on analytic solutions, we propose tensile stress and strain energy based criteria for the initiation and propagation of cracks in insertion electrodes. These criteria may help guide the development of new materials for lithium ion batteries with high energy density and long cycle life. We will also discuss self-healing and surface modification to enhance the performance and durability of lithium ion batteries.

Biography: Y.T. Cheng is the Frank J. Derbyshire Professor of Materials Science in the Department of Chemical and Materials Engineering at the University of Kentucky. His current research interests include synthesis, characterization, and modeling of materials for energy storage and biomedical applications. Prior to joining the faculty at Kentucky in the fall of 2008, he was a technical fellow and laboratory group manager for engineered surfaces and functional materials at the General Motors Research and Development Center in Warren, Michigan. He began his college education in physics at Peking University before transferring to the California Institute of Technology where he obtained his BS degree in physics with a minor in mathematics in 1982, and his MS and PhD degrees in applied physics in 1983 and 1987, respectively. He has authored or co-authored more than 140 publications and holds 46 US patents. He is a Fellow of the American Physical Society and a Fellow of the Materials Research Society. He is also a member of The Electrochemical Society and ASM International.