

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT COLLOQUIUM SERIES PRESENTS:

Stephan Hruszkewycz

Assistant Physicist, Argonne National Laboratory



Opportunities for materials science with coherent x-ray diffraction imaging

Recent progress in 3D coherent x-ray diffraction imaging methods can enable high resolution structural imaging of nano-structured crystalline materials under operating conditions. In this talk, I discuss developments in Bragg coherent diffraction imaging (BCDI) that aim to broaden the envelope of materials science problems that can be addressed with the technique. Following an introduction of the basic principles of the method, two specific topics will be discussed: 1) BCDI at high x-ray energies that provide dramatic penetrating ability, 2) Bragg ptychography that enable imaging of targeted sub-volumes of a crystal. Both approaches will be discussed in the context of materials science problems that can be addressed in-situ at next-generation synchrotron storage rings including the Upgraded Advanced Photon Source project now underway at Argonne National Laboratory.

Stephan Hruszkewycz is a staff scientist in the Materials Science Division at Argonne National Laboratory. His research focuses on developing and using coherent x-ray scattering techniques to interrogate nanoscale materials structure and dynamics under working conditions to reveal structure-property relationships. Currently he is using strain-sensitive coherent Bragg diffraction to image subtle strain fields in nanoscale crystals for photonic and quantum information applications. These research thrusts are pursued at high-brightness synchrotron sources with state-of-the-art coherence-preserving beamlines, including those at the Advanced Photon Source, NSLS-II, and LCLS, and aim to broaden the applicability of coherent diffraction imaging within both the broader materials science community.

Tuesday, September 25 • 4 pm •

Tech L211

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT COLLOQUIUM SERIES PRESENTS:

Yi Cui

Professor of Materials Science and Engineering
Stanford University

Stanford Institute for Materials and Energy Sciences, SLAC
National Accelerator Laboratory



Nanomaterials Design for Energy Storage and Catalysis

Nanomaterials and interfacial design affords a powerful approach in addressing the problems in energy conversion and storage. Here I will present a decade long research in my group in the area of energy storage and catalysis, including 1) materials design for overcoming volume expansion and interfacial instability of high capacity lithium battery materials including Si anodes, Li metal anodes and S cathodes; 2) new battery chemistries (Mn-H₂ aqueous batteries and solid-state molten batteries) for grid scale energy storage with low cost and long cycle life; 3) electrochemical and strain tuning of catalysts for HER, OER and ORR. 4) The development of cryogenic electron microscopy for materials science to unravel long-standing important materials science questions.

Yi Cui is a Professor in the Department of Materials Science and Engineering at Stanford University. He received B.S. in Chemistry in 1998 at the University of Science and Technology of China (USTC), Ph.D in 2002 at Harvard University. After that, he went on to work as a Miller Postdoctoral Fellow at University of California, Berkeley. In 2005 he became an Assistant Professor in the Department of Materials Science and Engineering at Stanford University. In 2010 he was promoted with tenure. His current research is on nanomaterials for energy storage, photovoltaics, topological insulators, biology and environment. He has founded three companies to commercialize technologies from his group: Amprius Inc., 4C Air Inc. and EEnovate Technology Inc.

Tuesday, October 2 • 4 pm • Tech L211

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT COLLOQUIUM SERIES
PRESENTS:

Maryam Ghazisaeidi

Assistant Professor, Materials Science Engineering
Assistant Professor, Physics
Ohio State University



Tuesday, October 30 • 4 pm
Tech L211

High entropy alloys: mechanical properties and phase stability

The term “High entropy” alloys (HEA) refers to a relatively new class of multicomponent—usually five or more—metallic alloys in equal or near equal atomic concentrations. Instead of ordered intermetallics, expected from classical physical metallurgy, some HEA systems strikingly crystallize as single phase solid solutions with simple crystal structures. The complex compositions of these alloys, and their derivatives, lead to unique properties. They also encourage new ways of viewing fundamentals of physical metallurgy, yielding new insights that are applicable to a wide range of metallic alloys. In this talk I will present two aspects of these systems: mechanical properties and thermodynamics.

In the first part, I present a phase transformation strengthening mechanism in CrCoNi, a ternary derivative of the CrMnFeCoNi high entropy alloy. CrCoNi alloy exhibits a remarkable combination of strength and plastic deformation, even superior to the CrMnFeCoNi high-entropy alloy. We connect the magnetic and mechanical properties of CrCoNi, via a magnetically tunable phase transformation. While both alloys crystallize as single-phase face-centered-cubic (fcc) solid solutions, we find a distinctly lower-energy phase in CrCoNi alloy with a hexagonal close-packed (hcp) structure. Comparing the magnetic configurations of CrCoNi with those of other equiatomic ternary derivatives of CrMnFeCoNi confirms that magnetically frustrated Mn eliminates the fcc/hcp energy difference. This highlights the unique combination of chemistry and magnetic properties in CrCoNi, leading to a fcc-hcp phase transformation that occurs only in this alloy, and is triggered by dislocation slip and interaction with internal boundaries.

In the second part, I present our Multi-cell Monte Carlo (MC)² method for predicting stable phases of alloys from first principles calculations. Application of this method to the high entropy HfZrTaNbTi HEA, confirms the experimental observations of phase separation in this alloy and provides a powerful tool for predicting the thermodynamically stable phases of multicomponent alloys. In addition, our prediction of phase separation, in line with experiments, cast new doubts on the equilibrium stable phases of those HEAs which had been widely regarded as random solid solutions.

Maryam Ghazisaeidi is an assistant professor in the department of Materials Science and Engineering at Ohio State University. Her research interest is in the area of computational materials science at the atomic-scale with an emphasis on understanding structure and chemistry of defects in structural materials to predict novel material behavior. Dr Ghazisaeidi is the recipient of the NSF CAREER award in 2015 and the AFOSR Young Investigator Program (YIP) award in 2017. She received her B.S and M.S. from Sharif University of Technology in Tehran, Iran, and her Ph.D from the University of Illinois at Urbana-Champaign.

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT COLLOQUIUM SERIES PRESENTS:

Linsey Seitz

Assistant Professor of Chemical and Biological Engineering
Northwestern University

Oct. 23, 4pm Tech L211



Developing Enhanced Electrochemical Catalysts using Spectroscopic Insights

Renewable sources, such as wind and sun, supply more than enough energy to meet the increasing global demand and are promising solutions to shift our dependence away from fossil fuels as long as challenges with intermittency, scale, and cost effectiveness can be overcome. While recent developments have improved capture efficiencies for these sources, effective processes to convert and store this energy are needed. Chemical storage of energy using optimized catalytic reactions can produce high energy density fuels and commodity chemicals while allowing for spatiotemporal decoupling of the energy production and consumption processes. This talk will cover some recent work pursuing fundamental understanding of such catalytic reactions towards production of renewable fuels and chemicals as well as the vision for future activities of the new Seitz Lab at Northwestern. This work includes studies of controlled catalyst surfaces with an emphasis on determining intrinsic catalyst activity coupled with insights from advanced characterization techniques, such as x-ray absorption and x-ray emission spectroscopy, which are invaluable for investigating electronic, chemical, and geometric structure of materials.

Linsey Seitz received her B.S. (2010) in Chemical Engineering from Michigan State University supported with a full ride from the Alumni Distinguished Scholarship. Linsey received her M.S. (2013) and Ph.D. (2015) in Chemical Engineering from Stanford University under the guidance of Professor Thomas Jaramillo. During her graduate studies, Linsey was a National Science Foundation Graduate Research Fellow and a Stanford DARE Fellow; the latter is a fellowship program for advanced doctoral students who want to pursue academic careers and whose presence will help diversify the professoriate. Her research at the interface of catalysis and spectroscopy has taken her to a number of synchrotron facilities to conduct in situ studies, including the Stanford Synchrotron Radiation Lightsource in Menlo Park, CA, the Advanced Light Source in Berkeley, CA, and the KARA Synchrotron Radiation Source in Karlsruhe, Germany. In September 2018, Linsey joined Northwestern University's Chemical and Biological Engineering Department as a new Assistant Professor.

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT COLLOQUIUM SERIES PRESENTS:

Alix Deymier

Assistant Professor, Biomedical Engineering
UConn Health Center



Tuesday, November 6 • 4 pm
Tech L211

But Wait There's More!: How Musculoskeletal Tissues Resist Failure

Musculoskeletal injuries result in 65 million health care visits per year in the United States. The most common injuries are bone fractures and tendon tears or strains. In healthy musculoskeletal tissues, the body is able to decrease failure risks via complex hierarchical structures. These structures include composition gradients, energy absorbing and stress minimizing architectures, as well as multiphase composites. Disease, previous injury, and environmental factors, such as increased body acidity or muscle unloading, can modify the unique tissue structure and significantly increase failure risk and extent. To develop techniques for preventative and post-injury care it is therefore important to identify the musculoskeletal structures at multiple hierarchies and determine their mechanical roles. In addition, understanding these natural tissues can aid in the creation of new implants and devices. Alix Deymier has been investigating the role of architecture and composition from the nano- to the macro-scale on the mechanics of the musculoskeletal system via a variety of techniques including electron-energy loss spectroscopy, synchrotron x-ray diffraction, micromechanical testing, and microcomputed-tomography. She will present her work explaining how bones and tendons employ a hierarchy of structures and mechanisms to minimize failure and how these can be controlled and modified.

Alix Deymier, Ph.D., is currently an assistant professor in Biomedical Engineering at the UConn School of Dental Medicine. She is interested in studying the role of mineral composition, structure, and organization on the mechanics of mineralized biological tissue especially in the context of acid-base interactions in the body. Her interests focus on how pH modifying pathologies such as acidosis and unloading can affect bone structure and function at the nano-, micro-, and macro-scales. She was previously a postdoctoral fellow in Orthopedic Surgery at Columbia University and Washington University where she had an NSBRI fellowship studying the role of mineral structure and organization on the mechanics of biological systems in microgravity. She obtained her Ph.D. in Materials Science and Engineering at Northwestern University where she was a NDSEG and NSF Graduate Fellow working with High Energy X-ray Diffraction to study load transfer and mineral structure in mineralized biological systems. She completed her B.S. in Materials Science and Engineering at the University of Arizona in 2006 with a specialization in spectroscopy and the science of cultural heritage materials.

Oleg Gang

Professor

Department of Chemical Engineering and Department of applied Physics and Applied Mathematics, Columbia University

Tuesday, November 13 | 4 PM | Tech L211



Programmable Nano-Systems: form Designed Architectures to Controllable Processes

The ability to organize nano-components into the desired organizations is one of the major limitations for creating functional material systems. Our efforts are focused in establishing a broadly applicable DNA-based platform to address this challenge. DNA provides versatile means for interaction encoding, and much progress was achieved in the recent years in our ability to tailor DNA structures. However, it is challenging to prescribe the behavior of the entire nanoscale system, built from DNA and other biotic and abiotic components, and to translate advances in DNA structuring into a material design.

Our research explores approaches for creating targeted static and dynamic nano-architectures by bridging DNA-encoded nano-objects with structural plasticity and programmability of DNA macromolecular constructs. Through establishing assembly processes and revealing the principles governing systems with DNA-encoded interactions, we develop methods for creation of well-defined three-dimensional lattices, two-dimensional membranes and finite-sized clusters from the multiple types of the nano-components. Our recent progress demonstrates an integration of DNA with both inorganic and biological nanocomponents into well-defined objects, and a new platform for the formation of ordered materials with engineered organizations and compositions. Our current advances of using programmable assembly for a fabrication of targeted nanomaterials, and exploring their optical, mechanical, and chemical functions will be also discussed. Finally, as a next level of a system control, we investigate how to regulate dynamic processes in these self-assembled systems.

Oleg Gang is a Professor of Chemical Engineering, and of Applied Physics and Materials Science at Columbia University, and a Leader of Soft and Bio-Nanomaterial group at Brookhaven National Laboratory. His research explores the behavior of soft matter at the nanoscale and develops novel strategies for programmable assembly of targeted nanomaterial. Dr. Gang earned Ph.D. from Bar-Ilan University and was a postdoctoral Rothschild Fellow at Harvard University. He joined Brookhaven National Laboratory (BNL) as Distinguished Goldhaber Fellow in 2003, where he became a leader of Soft and Bio-Nanomaterials group at the BNL's Center for Functional Nanomaterials in 2008. Dr. Gang has joined Columbia faculty in 2016. His group develops new strategies for creating materials by design using self-assembly approaches, explores phenomena and properties of newly developed nanomaterials, as well as employs advanced in-situ probes for understanding a material formation. Gang has received numerous awards and recognitions, including Gordon Battelle Prize for Scientific Discovery and Department of Energy Outstanding Mentor Award, and he is a Fellow of American Physical Society.

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT COLLOQUIUM SERIES PRESENTS:

Xiaobing Hu

Research Assistant Professor, Northwestern University



Advanced Applications of TEM in Engineering Alloys

Because of the superior creep and oxidation resistance at high temperature, superalloys have a continued important role in high temperature materials applications such as gas turbines and power plants. As a microelement, boron (B) is generally added into almost all the commercial superalloys for strengthening the grain boundaries. Even for the single crystal superalloys, many low-angle grain boundaries still exist, where addition of suitable B is also very helpful to achieve good overall properties. B tends to segregate at the boundaries/interfaces as the solution state. Additionally, B also tends to form various kinds of boride (e.g. M₃B₂, M₂B, M₅B₃). As for the detailed microstructural features of these borides, there is limited knowledge in available literatures. Accurate understanding of these microstructural features is very helpful to discuss the structure-property relationship. Thus, in the past 10 years, we performed a systematical study on above borides by means of various microscopy methods based on the aberration corrected TEM. In this talk, I will introduce the advanced applications of TEM methods on revealing the atomic scale structural and chemical features of these borides.

Dr. Xiaobing Hu is a research assistant professor in the Department of Materials Sciences and Engineering at Northwestern University. He received his B.S. in Materials Sciences and Engineering from Central South University in China in 2009. He received his Ph.D. from Institute of Metal Research, Chinese Academy of Sciences (IMR, CAS) in 2015 for studies of electron microscopy and its advanced applications in superalloys supervised by Prof. Xiuliang Ma. After that, he worked as a postdoc researcher supervised by Prof. Yuichi Ikuhara at Japan Fine Ceramic Center (JFCC). Then, he joined Brookhaven National Laboratory (BNL) as a research associate supervised by Dr. Yimei Zhu. Xiaobing joined NUANCE center in August 2018. His interest is the advanced applications of various TEM methods in materials science. During the past 10 years, he has been focusing the research work on various engineering alloys and energy storage materials.

Tuesday, January 8 • 4 pm • Tech L211

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT COLLOQUIUM SERIES PRESENTS:

Samantha Daly

Professor, Department of Mechanical Engineering
University of California, Santa Barbara



Machine Learning and Computer Vision for Deformation Mechanism Analysis

The influence of microstructure on deformation and failure mechanisms, such as twinning, slip, grain boundary sliding, and multi-crack systems, includes complex stochastic and deterministic factors whose interactions are currently under active debate. In this talk, the application of machine learning and computer vision to microscale displacement data for the segmentation and identification of deformation mechanisms – in this example, deformation twinning in magnesium – and their evolution under load across mm-scale fields of view is discussed. A recently developed experimental approach to obtain high-resolution, large FOV microscale deformation maps is presented, obtained using a combination of scanning electron microscopy and digital image correlation, aided with chemically-functionalized nanoparticle assembly for speckle patterning and external codes for improved electron beam scan control, test automation, and experimental analysis. The newly developed experimental and analytical approaches are length scale independent and material agnostic, and can be modified to identify a range of deformation and failure mechanisms. The advantages and disadvantages of various large data analysis approaches will be discussed, where the balance between computational cost and incurred error are considered.

Sam Daly is an Associate Professor in the Department of Mechanical Engineering at the University of California at Santa Barbara. She received her Ph.D. from Caltech in 2007 and subsequently joined the University of Michigan, where she was on the faculty until 2016 prior to her move to UCSB. Her interests lie at the intersection of experimental mechanics and materials science, with an emphasis on using novel methods of experimentation coupled closely with theoretical and computational modeling. Group research focuses on the statistical quantification of microstructural features of materials and their effect on meso- and macro-scale properties. Currently, the group is engaged in the development of novel methods of multi-scale material characterization, with application to structural metallic alloys, active materials, advanced composites, high cycle and dwell fatigue mechanisms, plasticity, fracture, and material behavior at the microscale. Her recognitions include the NSF CAREER Award, the ASME Eshelby Mechanics Award, the Journal of Strain Analysis Young Investigator Award, the Experimental Mechanics Best Paper of the Year Award, the IJSS Best Paper of the Year Award, the DOE Early Career Award, the AFOSR-YIP Award, the ASME Orr Award, and the Caddell Award.

Tuesday, January 15 • 4 pm • Tech L211

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT COLLOQUIUM SERIES PRESENTS:

Shrikant Bhat

Senior Principal Scientist, ArcelorMittal Global R & D.



Cyclic Stability and Strain Localization during Fatigue of Advanced High Strength Steels

Cycle dependent changes in deformation resistance have been challenges in both engineering design of structures and new steel grade development for almost 200 years. Newer Advanced High Strength Steel (AHSS) grades with higher Tensile strength and ductility are being developed at an ever increasing pace utilizing a combination of metallurgical strengthening mechanisms. Many of these alloy designs often result in challenges to meet the implementation requirements from “end-use” and “in-use” perspectives, including component durability. This seminar will highlight two related aspects in developing fatigue resistant steel grades. First, cycle dependent changes in deformation resistance of several commercial steel grades will be illustrated with special emphasis on the role of the second phase in a ferrite matrix. The second aspect refers to how a slip line develops into a crack from cyclic deformation over many thousands of cycles. It is well known that strain localization leads to the formation of Persistent Slip Bands (PSBs) which eventually become fatigue cracks. The role of the second phase particles that impart static strengthening, especially martensite/bainite, in strain localization and the evolution of PSBs will be illustrated through quantitative stereological observations. These semi-empirical models indicate that reducing strain localization is beneficial for improved fatigue resistance. Utilization of these concepts in commercial steel grade development will also be highlighted.

Dr. Shrikant P. Bhat is a Senior Principal Scientist at ArcelorMittal Global R&D, East Chicago, IN. He obtained his Ph. D. (1978) in Metallurgy and Materials Science from the University of Pennsylvania, Philadelphia and continued as a Post-Doctoral fellow. He joined the former Inland Steel R&D Center in early 1979 and has enjoyed working in a variety of challenging positions both within Research and Steel Manufacturing. He has held various managerial positions and has worked extensively with customer R&D Centers in advanced engineering phases. His research interests have spanned cyclic deformation and fatigue, hydrogen susceptibility, deformation modelling and many other aspects related to steel usage. He has been an Adjunct Professor at Purdue University Northwest, and a Guest Lecturer at the Stronach Center for Innovation, University of Toronto. He has served on many thesis committees and was a Co-Principal Investigator for the Inland Steel – Northwestern University cooperative research program funded by NSF. He has won several awards, including the Michael C. Tenenbaum Award for the Best Paper, Inland Steel Chairman’s awards, and the Electron Microscopy Society of America Presidential Scholarship.

Tuesday, January 22 • 4 pm • Tech L211

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT COLLOQUIUM SERIES PRESENTS:

Roberto dos Reis

Research Assistant Professor, Northwestern University



Probing Properties of Matter at the Nanoscale by Using Scanning Electron Diffraction

The fundamental pillars of emergent physics and functionality of materials lie in the structural complexity of the atomic constituents. A complete understanding of this complex correlation requires experimental methods that are able to deliver a direct relationship between the properties and the atomic structure. However, the experimental determination of materials properties at nanoscale is often challenging and requires techniques that combine high spatial resolution, precision, and chemical sensitivity. In this colloquium, I will show examples of how to explore the information contained in the transmitted scattering of a finely focused electron beam traversing a thin foil. The resultant convergent beam electron diffraction (CBED) patterns include localized information on sample structure, composition, phonon spectra, three-dimensional defect crystallography and more. Recent advances in the fast-pixelated detector technology have enabled collection of these CBED patterns at many probe positions with millisecond dwell times, namely scanning electron diffraction. As a result, many image modalities can be achieved from a single dataset. I will demonstrate the usefulness of this technique to solve materials problems including precisely determination of octahedral rotation in electron beam sensitive halide-based perovskites using ptychography, local symmetry in ferroelectric ultra-thin films, three-dimension polarization in perovskites oxides, and more. Additionally, strategies for handling, processing and extracting useful data from such large datasets will be addressed.

Dr. Roberto dos Reis is specialized in advanced characterization of a vast range of materials using transmission electron microscopy (TEM) techniques. He has B.Sc, M.Sc and Ph.D degrees in Physics from Federal University of Rio Grande do Sul in Brazil where he worked on synthesis and characterization of semiconductor thin-films. During his PhD studies, he was a long-term visiting scholar at Lawrence Berkeley National Laboratory (LBNL)/CA working under supervision of Dr. Zuzanna Liliental-Weber on characterizing highly mismatched III-V and II-V semiconductor alloys for photovoltaic applications as member of the electronic materials group from 2010-2013. In the last 5 years, Roberto worked alongside Dr. Ulrich Dahmen and Dr. Jim Ciston as postdoctoral researcher at the National Center for Electron Microscopy (NCEM) facility of the Molecular Foundry/LBNL applying advanced electron diffraction techniques to a variety of materials as well as collaborating with several users in a multidisciplinary environment.

Tuesday, January 29 • 4 pm • Tech L211

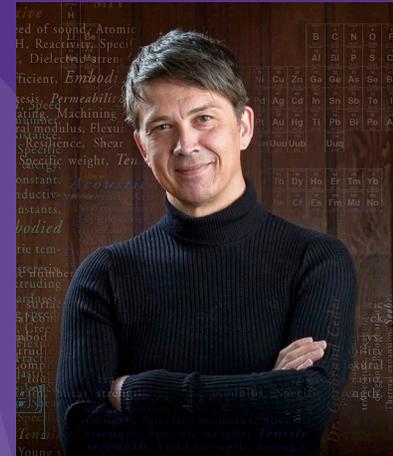
THE MATERIALS SCIENCE & ENGINEERING DEPARTMENT SEMINAR SERIES PRESENTS:

2019 Morris E. Fine Lecture

Gerbrand Ceder, PhD

Daniel M. Tellep Distinguished Professor in Engineering • University of California, Berkeley

Gerbrand Ceder's research interests lie in computational and experimental materials design for clean energy technology and in Materials Genome approaches to materials design and synthesis. He has published over 400 scientific papers, and holds more than 25 U.S. and foreign patents. He is a member of the National Academy of Engineering of the US and the Royal Flemish Academy of Belgium for Science and The Art. He is a Fellow of the Materials Research Society and the Metals, Minerals and Materials Society, and has received awards from the Electrochemical Society, the Materials Research Society, the Metals Minerals and Materials Society, and the International Battery Association. He is a co-founder of Computational Modeling Consultants, Pellion Technologies, and The Materials Project.



Tuesday, February 5 • 4 pm | Tech L211

Reception • 5pm | Willens Wing Atrium

Northwestern | McCORMICK SCHOOL OF ENGINEERING

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT
COLLOQUIUM SERIES PRESENTS:

Elsa Olivetti

Atlantic Richfield Associate Professor of Energy Studies
in the Department of Materials Science and Engineering,
MIT



Text and Data Mining for Material Synthesis.

Predictive materials modeling can provide properties of real and virtual compounds and will be available on demand, thereby enabling rapid iteration time in materials design. However, the allure (and necessity) of accelerated discovery that motivates computational materials design is diminished by the prevalent heuristic approaches to materials synthesis and optimization. This delay in moving from promising materials concept to validation, optimization, and scale-up is a significant burden to commercialization. I will describe our work to extract information from peer reviewed academic literature across a range of inorganic solid state materials synthesis approaches. We have demonstrated not only the potential of the natural language processing (NLP) approach to assemble materials data from the literature, but we have also shown that one can develop hypotheses for what synthesis conditions drive a particular target material outcome using learning approaches.

Elsa Olivetti is the Atlantic Richfield Associate Professor of Energy Studies in the Department of Materials Science and Engineering. Her research focuses on improving the environmental and economic sustainability of materials using methods informed by materials economics, machine learning, and techno-economic analysis. She has received the NSF Career award for her experimental research focused on beneficial use of industrial waste materials. Dr. Olivetti received her B.S. degree in Engineering Science from the University of Virginia. Her Ph.D. in Materials Science and Engineering from MIT was focused on development of cathode materials for lithium ion batteries.

Tuesday, February 12 • 4 pm | Tech L211

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT COLLOQUIUM SERIES PRESENTS:

Joseph P. Heremans

Ohio Eminent Scholar and Professor in the Mechanical and Aerospace Engineering Department, Ohio State University



Entropy transport in Weyl Semimetals

The last decade has seen a research focus on the electronic properties of materials with topological qualities. The spectrum of the electron excitations in these materials is characterized by topological invariants. Topological invariants are properties that do not change under continuous changes of quantities, such as interaction strengths, except when some symmetry or related transition occurs. These invariants control the number and nature of the surface and edge states in topological insulators (TIs) and bulk states in Weyl and Dirac semimetals.

Convincing evidence for the existence of these states comes from angular resolved photoelectron spectroscopy (ARPES), but real applications must involve electronic transport properties. Electrical conductivity and Hall Effect measurements face experimental difficulties. In this talk, emphasis will be put on thermal transport properties, namely electronic thermal conductivity and the Seebeck and Nernst effects. We posit that thermal transport provides some of the simplest and most convincing evidence of the effect of chirality and protection on the transport properties of Weyl semimetals.

Heremans is an Ohio Eminent Scholar and Professor in the Mechanical and Aerospace Engineering Department at the Ohio State University, with appointments in the Materials Science and Engineering Department and the Department of Physics. He is a member of the National Academy of Engineering, and a fellow of AAAS and the American Physical Society. He joined OSU after a 21 year career in the automotive industry at the General Motors Research Laboratories, where he was the section manager for Semiconductor Physics, and at the Delphi Research Laboratories. His research interests focus on energy conservation and recovery, and lie at the intersection between experimental condensed matter physics and thermodynamics. In the last decade, he worked on the transport of heat, charge, and magnetization in solids.

Tuesday, February 19 • 4 pm | Tech L211

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT SPRING COLLOQUIUM SERIES PRESENTS:

Enrique Martinez Saez

Staff Scientist, Los Alamos National Laboratory



The Kinetic Monte Carlo Algorithm in Materials Science: Study of Radiation-Induced Segregation in Fe-Cr alloys

In this talk I will describe the details of the kinetic Monte Carlo (KMC) algorithm, the theory behind it and its relation with the Markovian master equation. I will then focus on its application to alloy systems under irradiation and how it can model those systems far from equilibrium. Nonequilibrium chemical redistribution in open systems submitted to external forces, such as particle irradiation, leads to changes in the structural properties of the material, potentially driving the system to failure. Such redistribution is controlled by the complex interplay between the production of point defects, atomic transport rates, and the sink character of the microstructure. We have recently developed an interaction model for the Fe-Cr system that incorporates physically accurate thermodynamic driving forces and kinetic coefficients. We have employed this model to analyze the afore-mentioned interplay between alloying elements and irradiation-created defects to study the effect of ideal defect sinks on Cr concentration profiles, with a particular focus on the role of interface density. We observe that the amount of segregation decreases linearly with decreasing interface spacing. Within the framework of the thermodynamics of irreversible processes, a general analytical model is derived and assessed against the KMC simulations to elucidate the structure-property relationship of this system. Interestingly, in the kinetic regime where elimination of point defects at sinks is dominant over bulk recombination, the solute segregation does not directly depend on the dose rate but only on the density of sinks. This model provides new insight into the design of microstructures that mitigate chemical redistribution and improve radiation tolerance.

Dr. Enrique Martinez Saez is a staff scientist at the Los Alamos National Laboratory (LANL), in the Theoretical division. He is the team lead expert on Monte Carlo and Dislocation Dynamics methods applied to materials science and heavily involved in atomistic approaches. Prior to Dr. Saez's current position at LANL, he worked at the Madrid Institute for Advanced Studies of Materials (IMDEA) as a Junior Researcher. Dr. Saez's research interests lie on the study of the microstructural evolution of materials under extreme conditions of irradiation, temperature and deformation and its relation to the macroscopic system response. The design of advanced materials is crucial in the quest for cleaner, more efficient energy sources. Theoretical developments along with modeling and simulation strategies, which Dr. Saez devotes his research to, have become paramount in this quest, to guide and interpret experimental approaches.

Tuesday, April 2 • 4 pm • Tech L361

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT SPRING
COLLOQUIUM SERIES PRESENTS:

Junqiao Wu

Professor of Materials Science and Engineering
University of California, Berkeley



When quantum materials get hot: anomalous thermal conduction and radiation

Heat conduction in and radiation from solids provides a unique window to probe solid state physics, and also plays a pivotal role for a wide range of industry applications. Although it is a traditional research focus in mechanical engineering, study of heat transfer from materials scientists' perspective would result in new discovery, new insight and new applications.

In this talk, I will show our recent work on understanding novel charge dynamics and electron-phonon interactions of quantum materials with electronic phase transitions. An unusually low electronic thermal conductivity is found in metallic vanadium dioxide, and is a signature of absence of quasiparticles in a strongly correlated electron fluid where heat and charge diffuse independently. An unusual, temperature-independent lattice thermal conductivity is found in crystalline tantalum disulfide, which is attributed to strong electron-phonon coupling that dominates over the conventional phonon-phonon scattering.

I will also discuss how we engineer these materials for novel thermal applications. By grading or meta-structuring the metal-insulator phase transition, we demonstrate temperature-independent thermal radiation which is used for a superior infrared camouflage and decoy, as well as switchable thermal radiation which is used for smart radiative cooling.

Professor Junqiao Wu received a B.S. from Fudan University and a M.S. from Peking University, China. He obtained a Ph.D. degree from the University of California, Berkeley, and did postdoctoral research at Harvard University. He is currently a professor at the Department of Materials Science and Engineering, and the Chair of the Applied Science and Technology Graduate Group at UC Berkeley, and also holds joint appointment at the Lawrence Berkeley National Laboratory. His honors include the 29th Ross N. Tucker Memorial Award, the US-NSF Career Award, the US-DOE Early Career Award, the Presidential Early Career Award for Scientists and Engineers (PECASE) from the White House, the Outstanding Alumni Award from Peking University China, and the Fellow of APS. The Wu group explores novel properties and applications of nanomaterials, phase transitions at the nanoscale, and optoelectronic, thermal and thermoelectric properties of electronic materials. Prof. Wu has published over 200 widely cited papers in these fields.

Tuesday, April 9 • 4 pm | Tech L361

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT SPRING COLLOQUIUM
SERIES PRESENTS:

Prineha Narang

Professor, Harvard University



Correlated Light-Matter Interactions and Excited-State Dynamics in Quantum Materials

The physics of quantum materials is rich with spectacular excited-state and non-equilibrium effects, but many of these phenomena remain poorly understood and consequently technologically unexplored. Therefore, this talk will focus on how quantum-engineered materials behave, particularly away from equilibrium, and how we can harness these effects in quantum technologies and quantum information science. Electron-photon, electron-electron as well as electron-phonon dynamics and far-from-equilibrium transport are critical to describe ultrafast and excited-state interactions in materials. Ab initio descriptions of phonons are essential to capture both excitation and loss (decoherence) mechanisms, and are challenging to incorporate directly in calculations due to a large mismatch in energy scales between electrons and phonons. I will show results using a new theoretical method we have developed to calculate arbitrary electron-phonon and electron-optical interactions in a diagrammatic many-body framework integrated with a nonequilibrium carrier transport method. Further, I will discuss a new formalism at the intersection of cavity quantum-electrodynamics and electronic structure methods, quantum-electrodynamical density functional theory, to treat electrons and photons on the same quantized footing. I will demonstrate how these ab initio techniques guide the search for relevant quantum properties in 2D and 3D materials, including new quantum emitters. Finally, I will show recent results using newly developed theoretical methods to evaluate the linear and nonlinear optical properties of low dimensional and heterostructured quantum materials and pathways to leverage these properties in quantum devices.

Prineha Narang is a Professor at the John A. Paulson School of Engineering and Applied Sciences at Harvard University. Prineha's work has been recognized by many awards and special designations, including being named a Moore Inventor Fellow by the Gordon and Betty Moore Foundation for innovations in quantum science and technology, CIFAR Azrieli Global Scholar by the Canadian Institute for Advanced Research, a Top Innovator by MIT Tech Review (MIT TR35), and a Young Scientist by the World Economic Forum in 2018. In 2017, she was named by Forbes Magazine on their "30under30" list for her work in atom-by-atom quantum engineering. Prineha designs materials at the smallest scale, using single atoms, to enable the leap to quantum technologies. She has pioneered work in classical and quantum computing to approach problems in physics and chemistry with a new toolkit. At SEAS she designed and teaches ES 170, a popular undergraduate class on quantum engineering. Outside of science, she is an avid triathlete and runner.

Tuesday, April 16 • 4 pm | Tech L361

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT SPRING COLLOQUIUM SERIES
PRESENTS:

Yang Shao-Horn

W.M. Keck Professor of Energy, MIT



Energy Storage Using Electrochemistry

Electrochemistry is used widely today, spanning from production of hydrogen and metals such as aluminum, and Li-ion batteries. We will discuss challenges and opportunities in using electrochemistry to store cheap electrons in materials and molecules with energy from the Sun. Recent learnings towards establishing design principles in controlling electrocatalysis, and ion mobility, central to the functions of electrochemical devices, will be presented.

Professor Shao-Horn is W.M. Keck Professor of Energy at the Massachusetts Institute of Technology (M.I.T.). Her research is centered on exploiting chemical/materials physics to understand and control kinetics and dynamics at interface and in bulk for energy storage and making of sustainable fuels. Professor Shao-Horn is a member of National Academy of Engineering and is among the World's Most Influential Scientific Minds and Highly Cited Researchers.

Tuesday, April 30 • 4 pm | Tech L361

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT SERIES PRESENTS
THE 2019 JOHN E. DORN MEMORIAL LECTURE



Karin Rabe, PhD

Professor of Physics
Rutgers, the State University of New Jersey

Functional Materials from First Principles

New materials can solve many (though not all) of the world's problems through faster, smaller-scale and cheaper processing and storage of information and energy. Improving and optimizing the materials we already use for these purposes can only take us so far -- what about something really new? How would we know where to look? Information about the structures and properties of experimentally known materials, as organized into a crystallographic database, provides the initial data for a rough map of the space of possible materials. Using the theory of quantum mechanics to perform first-principles computer simulations of the properties of known and as-yet hypothetical materials from first principles, using only their chemical composition as input, we can augment the database with the results of computer experiments to develop the map. Drawing on the unique capability of first-principles calculations to identify low-energy metastable states in addition to the equilibrium phase, we can predict phase transitions and functional properties "de novo": that is, without prior experimental clues. Several examples of such predictions for functional behavior in binary oxides, perovskites and ternary intermetallics will be presented. The challenges and promise of theoretical materials design and theoretical-experimental integration will be discussed.

Karin Rabe is a computational materials physicist with a particular interest in the use of first-principles quantum-mechanical calculations for the study of phase transitions and the theoretical design of new materials. Born in New York City, she attended the Bronx High School of Science and majored in physics at Princeton University. She received a Ph.D. in physics from Massachusetts Institute of Technology (1987) with thesis supervisor John Joannopoulos. Following two postdoctoral years in the theory department at AT&T Bell Laboratories, she joined the Department of Applied Physics and the Department of Physics at Yale University, with tenure in 1995, and moved to the Department of Physics and Astronomy at Rutgers in 2000, where she was promoted to Board of Governors professor of physics in 2013. She served as president of the Aspen Center for Physics from 2013 to 2016. Her recent professional recognition includes fellowship in the American Physical Society (2003), the David Adler Lectureship Award in the Field of Materials Physics from the American Physical Society (2008), fellowship in the American Association for the Advancement of Science (2011) and membership in the American Academy of Arts and Sciences (2013) and the National Academy of Sciences (2013).

Tuesday, May 21 • 4 pm Pancoe Auditorium
Reception to follow | Pancoe Cafe

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT SPRING COLLOQUIUM SERIES
PRESENTS:

Karen I. Winey

Department Chair, Professor and TowerBrook
Foundation Faculty Fellow of Materials Science and
Engineering, University of Pennsylvania

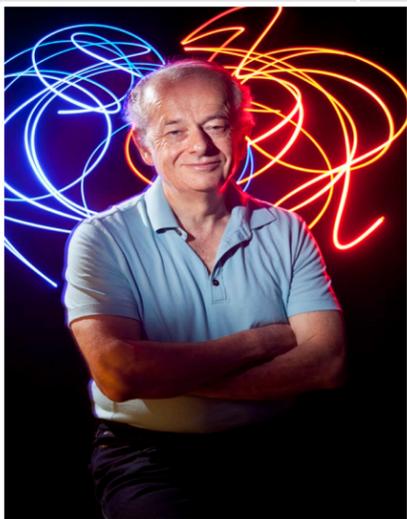


Precise Polymers that Control Nanoscale Morphologies & Transport Properties

Acid- and ion-containing polymers have specific interactions that produce acid- or ion-rich aggregates arranged in hierarchical nanoscale morphologies and remarkable bulk properties. Untangling the correlations between the primary structure of such associating polymers and their morphologies and properties has long been a challenge in polymer physics, because most acid- and ion-containing polymers have random sequences of polar and non-polar monomeric units. New synthetic methods increasingly produce polymers with greater molecular precision that provide greater uniformity of and control over the hierarchical morphologies. Using primarily X-ray scattering experiments and atomistic molecular dynamics simulations, we have revealed a variety of new nanoscale morphologies in precise acid- and ion-containing polymers (layers, branched aggregates, gyroid). In addition to describing these new morphologies, this seminar will present proton and ion conductivity results for a variety of precise polymers that demonstrate the importance of these new nanoscale morphologies.

Karen I. Winey received her B.S. from Cornell University in materials science and engineering and her Ph.D. in polymer science and engineering from the University of Massachusetts, Amherst. Following a postdoctoral position at AT&T Bell Laboratories, she joined the faculty of the University of Pennsylvania in 1992. Karen characterizes and manipulates nanoscale structures in ionomers and associating polymers to develop materials with improved mechanical and transport properties. Recently, she discovered new structures in several acid- and ion-containing precise polyethylenes. Karen also designs and fabricates polymer nanocomposites to understand and improve their mechanical, thermal, and electrical properties, particularly transparent conductors. Polymer motion in the presence of nanoparticles and in nanoconfinement are currently areas of interest. Across these research areas, Karen couples experimental studies with simulation and theory, either within her group or with collaborators. Karen has served the research community as Chair of the Division of Polymer Physics within the American Physical Society (2013) and as Chair of the Polymer Physics Gordon Research Conference (2010). Winey also served as an Associate Editor for *Macromolecules* (2010-14), the leading journal in the field. Karen has numerous honors including Fellow of the American Physical Society (2003), George H. Heilmeier Faculty Award for Excellence in Research (2012), Fellow of the Materials Research Society (2013), Visiting Miller Research Professor at the University of California, Berkeley (2014), Fellow of the PMSE Division within the American Chemical Society (2016) and the Trustees Council of PennWomen Award for Undergraduate Advising (2018).

Tuesday, May 28 • 4 pm | Tech L361



Federico Capasso

Robert L. Wallace Professor of Applied Physics
Vinton Hayes Senior Research Fellow in Electrical Engineering
Harvard John A. Paulson School of Engineering and Applied Sciences
Harvard University

Monday, June 3 • 4 pm Tech LR3
Reception to follow | Willens Wing Atrium

Talk 1: Flat optics: Overcoming the limits of refractive and Fresnel Optics

Sub-wavelength scale artificially structured dielectric surfaces, known as metasurfaces, enable the redesign of optical components such as lenses into thin, planar, and multifunctional elements. This leads to a major reduction in thickness, footprint, and system complexity, and leads to ease of optical alignment and aberration control. As well, this leads to the introduction of new optical functions, thus circumventing the limitations of refractive and conventional diffractive optics. The planarity of flat optics facilitates the unification of semiconductor manufacturing and lens-making, where the planar technology to manufacture chips will be adapted to make CMOS compatible metasurface-based optical components for high volume markets and for a wider range of specialty applications.

Tuesday, June 4 • 4 pm Tech Ryan Auditorium

Talk 2: Multifunctional Flat Optics

Metasurfaces enable arbitrary control of the wavefront of light by locally manipulating polarization in addition to amplitude and phase. As a result, multiple optical functions can be encoded with greatly reduced complexity that be accessed by changing the input polarization, wavelength and k-vector. Unique ways to generate structured light, a new polarization optics that greatly surpasses the capabilities of the standard and a new class of lenses that correct aberrations without requiring multiple stacked lenses have emerged from this approach. I will present spin-to-total angular momentum converters (J-plates) that create complex entangled states with applications in quantum optics and other fields, new polarimeters and polarization state generators and broadband achromatic lenses

Federico Capasso is a leader in nanophotonics and principal contributor to metasurfaces and Flat Optics since their beginnings. He pioneered bandgap engineering of artificially structured semiconductors which led him and his collaborators to the invention and development of the quantum cascade laser. He carried out fundamental studies of the Casimir effect including the first measurement of the repulsive Casimir force. He is the Robert Wallace Professor of Applied Physics at Harvard University, which he joined in 2003 after 27 years at Bell Labs where his career advanced from postdoctoral fellow to VP for Physical Research. He is a member of the National Academy of Sciences, the National Academy of Engineering and a fellow of the American Academy of Arts and Sciences (AAAS) and the National Academy of Inventors. He is the recipient of numerous international awards such as the Balzan Foundation Prize in Applied Optics, the King Faisal International Prize for Science, the Rumford Prize of AAAS, the Arthur Schawlow Prize of The American Physical Society (APS), the IEEE Edison Medal, The Optical Society of America (OSA) Wood Prize; the SPIE gold Medal, the Wetherill Medal of the Franklin Institute and the Materials Research Society Medal. He is a Fellow of the OSA, the IEEE, and the APS.