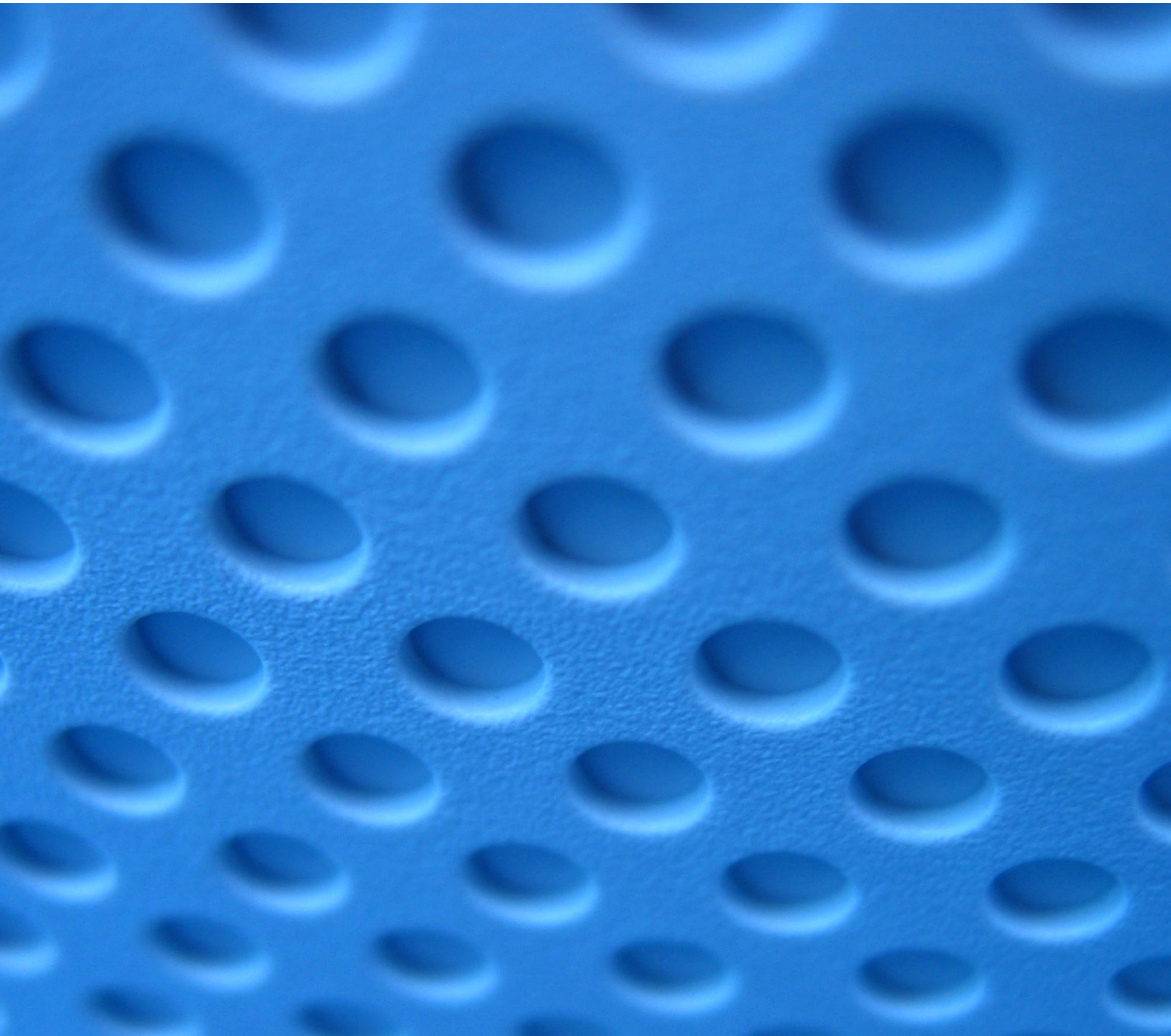
mpc 30+

advancing materials research

materials processing center

# Materials Day

## Computational Materials



## Materials Resources:

Materials Processing Center provides an environment where students and professionals from industry, government, and academia collaborate to identify and address pivotal multidisciplinary issues in materials processing and manufacturing at MIT.
http://mpc-web.mit.edu

Microphotonics Center @ MIT builds interdisciplinary teams, focused on collaborative research for the advancement of basic science and emerging technology pertaining to integrated photonic systems.
http://mphotonics.mit.edu

The Communications Technology Roadmap (CTR) is a project under the Microphotonics Industry Consortium, which in turn is part of the MIT Microphotonics Center. The purpose of this Roadmap is to understand the interaction between technology, industry, and policy dynamics and from there, formulate a vision for the future of the microphotonics industry.
http://mph-roadmap.mit.edu/

The Solid State Solar-Thermal Energy Conversion Center ($S^3$TEC) objective is to create novel solid-state materials for the conversion of sunlight and heat into electricity.
http://s3tec.mit.edu

Materials@MIT is a portal website to all materials activities at MIT.
http://materials.mit.edu

Center for Materials Science & Engineering is devoted to the design, creation, and fundamental understanding of materials that are capable of enhancing the human experience.
http://mit.edu/cmse

Department of Materials Science & Engineering is known as the world-wide leader in its field, pioneering advances in engineering sciences and technologies .
http://dmse.mit.edu

## Dates for future Materials Day Events:

Wednesday, October 17, 2012

Wednesday, October 23, 2013

MASSACHUSETTS INSTITUTE OF TECHNOLOGY

**MATERIALS PROCESSING CENTER**

*Materials Day at MIT*

# Computational Materials

October 18, 2011

Computational Materials will be the focus of this year's Materials Day. Computational methods have reached the point at which predictions of materials structures and properties can be made before they are demonstrated in the laboratory.  This has led to new breakthroughs in materials design that have greatly accelerated the development of new materials and processes that are optimized for a wide range of applications. Materials Day activities will include a one-day conference featuring speakers from both inside and outside MIT. A student poster session will follow featuring 50 to 100 posters with up-to-the minute research results from the broad materials research communities in MIT's Schools of Engineering and Science.

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Room 12-007
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## Materials Day Agenda

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|---|---|
| 8:00 am | **Registration** (Kresge Auditorium) |
| 8:45 am | **Welcome**<br>Professor Carl V. Thompson<br>Director, Materials Processing Center<br>Department of Materials Science & Engineering, MIT |
| **Session I:** | Professor Gerbrand Ceder<br>Session Chair<br>R. P. Simmons Professor of Materials Science and Engineering<br>Department of Materials Science & Engineering, MIT |
| 9:00 am | **The Yin and Yang of Computational Materials Design**<br>Dr. Sadasivan Shankar<br>Sr. Principal Engineer & Program Leader Materials Design<br>Intel Corporation |
| 9:40 am | **Atomic-Scale Modeling for the 21st Century Energy Challenges**<br>Professor Jeffrey C. Grossman<br>Carl Richard Soderberg Associate Professor of Power Engineering<br>Department of Materials Science & Engineering, MIT |
| 10:20 am | **Break** |
| **Session II:** | Professor Jeffrey C. Grossman<br>Session Chair<br>Carl Richard Soderberg Associate Professor of Power Engineering<br>Department of Materials Science & Engineering, MIT |
| 10:40 am | **Atoms to Airplanes: Simulation, Testing and the Future of Design**<br>Dr. Gerould K. Young<br>Director, Materials & Fabrication Technology<br>Boeing |
| 11:20 am | **From Atoms to Structures, Turning Weakness to Strength**<br>Professor Markus J. Buehler<br>Laboratory for Atomistic and Molecular Mechanics (LAMM)<br>Esther and Harold E. Edgerton Associate Professor of Civil and Environmental Engineering, MIT |

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| 12:00 - 1:00 pm | **Lunch**<br>Student Center, 3rd floor, Twenty Chimneys /Mezzanine Lounge (Bldg. W20) |
| **Session III:** | Dr. Sadasivan Shankar<br>Session Chair<br>Sr. Principal Engineer & Program Leader Materials Design<br>Intel Corporation |
| 1:10 pm | **Computational Materials Design - From Hard Coatings to Soft Membranes**<br>Dr. Yue Qi<br>Staff Research Scientist<br>Chemical Sciences and Materials Processes Lab<br>General Motors R & D and Planning |
| 1:50 pm | **The "Materials Genome" Project: Accelerated and Large-Scale Materials Discovery through Computation**<br>Professor Gerbrand Ceder<br>R.P. Simmons Professor of Materials Science and Engineering<br>Department of Materials Science & Engineering, MIT |
| 2:30 pm | **Soft Materials *in Silico:* Opening New Frontiers in Materials Science**<br>Professor Alfredo Alexander-Katz<br>Department of Materials Science & Engineering, MIT |
| 3:10 pm | **Wrap-up and Discussion with Attendees** |

**Materials Research Review Poster Session**

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| 3:30 pm | **Poster Session and Social**<br>La Sala De Puerto Rico, 2nd Floor Stratton Student Center (Bldg. W20) |
| 5:45 pm | **Poster Awards** |
| 6:00 pm | **Adjourn** |

# Professor Carl V. Thompson

**Director, Materials Processing Center**
**Stavros Salapatas Professor of Materials Science and Engineering, MIT**

## Biography

Professor Thompson received his SB in Materials Science and Engineering from the Massachusetts Institute of Technology in 1976. He received his SM and PhD degrees in Applied Physics from Harvard University in 1977 and 1982 respectively. He was an IBM postdoctoral fellow in the Research Laboratory of Electronics at MIT in 1982 and joined the faculty of the Department of Materials Science and Engineering in 1983. He is currently the Stavros Salapatas Professor of Materials Science & Engineering. Professor Thompson spent the 1990-91 academic year at the University of Cambridge Department of Materials Science and Metallurgy, where he was awarded a United Kingdom Science and Engineering Research Council Visiting Fellowship. He spent the 1997-98 academic year at the Max-Plank Institute fur Metallforschung in Stuttgart, Germany as a result of having received an award for Senior U.S. Scientist from the Alexander Von Humboldt Foundation. He was the President of the Materials Research Society in 1996. At MIT, Prof. Thompson currently Co-Chairs the Singapore-MIT Alliance program in Advanced Materials for Micro and Nano-Systems and is the Co-Director of the Iberian Nanotechnology Laboratory-MIT Program. He became the Director of the Materials Processing Center in 2008.


# Dr. Sadasivan Shankar

**Sr. Principal Engineer & Program Leader Materials Design**
**Intel Corporation**


## The Yin and Yang of Computational Materials Design


### Abstract

In the semiconductor industry, with the introduction of high-k & metal gate devices, materials have come to the forefront in addition to the transistor to enable Moore's law of scaling. Computational Materials Design (CMD) is recently associated with the concept of designing materials in silico for real materials applications. We will use specific cases in which CMD was successfully applied in synthesizing materials and in estimating properties. In addition, we will focus on critically evaluating the gaps in what is preventing from a successful application of CMD similar to Computational Fluid Dynamics, Structural, or Mechanical Design. We will conclude the talk by showing exciting opportunities for applications of chemistry, physics, and materials science in advancing the future generation of semiconductor process technologies


### Biography

Sadasivan Shankar is currently the Senior Principal Engineer and Program Leader for Materials Design, in the Design and Technology Group within the Intel Technology and Manufacturing Organization. In this thrust, his team works with experimentalists to enable computer-aided design of materials for addressing specific nanotechnology requirements. Over his tenure at Intel, he has worked on multiple aspects of technology development in Intel covering scales from atoms to architectures. Several areas in which his team's modeling facilitated technology adoption over 6 generations of scaling, have been recognized by several awards; flip chip packaging, advanced process control, dielectric engineering & integration, PMOS process optimization for strained transistor, polymer dielectric integration, and 100% Pb-free technology. He is the co-inventor in over 20 patent filings and co-author of over 75 external publications and presentations including 2 book chapters. Sadasivan earned his Ph.D in Chemical Engineering and Materials Science from University of Minnesota-Minneapolis.

In addition, Sadasivan is also actively involved in several new industrial and national research initiatives with National Institute of Standards and Technology, National Academies, National Science Foundation, Department of Energy, and several universities on materials-related research. Currently, the open platform effort that he has been involved in is part of President's new initiative on Materials Genome. Sadasivan is the Chair of Nanoengineered Materials Technical Advisory Board in Semiconductor Research Corporation and is on the Board of Advisors of University of Texas Austin-Chemical Engineering and Harvard University-Computational Science and Engineering.


# Professor Jeffrey C. Grossman

**Carl Richard Soderberg Associate Professor of Power Engineering**
**Department of Materials Science & Engineering, MIT**


## Atomic-Scale Modeling for the 21st Century Energy Challenges


### Abstract

One of the greatest challenges of the 21st century will be to understand, invent, and engineer new mechanisms and materials for energy production, energy storage and energy transport to counter the deleterious environmental and political impacts of our long-standing reliance on crude oil.  Current renewable energy conversion and storage technologies are too expensive, too inefficient, or both, substantially limiting their use and global impact. For example, over the last century we have used two trillion barrels of oil and are likely to retrieve and use another trillion in the next several decades. The sun provides that entire 3 trillion barrels worth of oil energy – in just 2 days. And yet, tapping into this enormous power to generate electricity is the least utilized renewable energy resource today. At the core of the energy challenge is a materials choice: many of the key mechanisms that convert and store energy are dominated by the intrinsic properties of the active materials involved. Our imperative is thus to predict, identify and manufacture new materials and designs as comprehensively and rapidly as possible, as the pressing challenge of producing and storing energy renewably calls for game-changing leaps forward rather than our current path of incremental advances. Toward that end, we use efficient atomic-scale computational approaches that serve both to elucidate fundamental mechanisms as well as predict completely new concepts and solutions. Our research focuses on the prediction of key properties that govern the conversion efficiency in these materials, including structural and electronic effects, interfacial charge separation, charge traps, excited states, band level alignment, and synthesis approaches. Examples of such calculations in the areas of solar photovoltaics and solar fuels will be presented.


### Biography

Jeffrey C. Grossman is the Carl Richard Soderberg Associate Professor of Power Engineering in the Department of Materials Science and Engineering at the Massachusetts Institute of Technology.  He received his Ph.D. in theoretical physics from the University of Illinois, performed postdoctoral work at U.C. Berkeley, and was a Lawrence Fellow at the Lawrence Livermore National Laboratory. He returned to Berkeley as Director of a Nanoscience Center and Head of the Computational Nanoscience research group with focus on energy applications, prior to joining MIT in Fall, 2009. Dr. Grossman's group uses theory and simulation to gain fundamental understanding, develop new insights based on this understanding, and then use these insights to develop new materials for energy conversion and storage with improved properties – working closely with experimental groups at each step. He has published more than 90 scientific papers on the topics of solar photovoltaics, thermoelectrics, hydrogen storage, solar fuels, nanomechanical phenomena, and self-assembly. He has appeared on a number of television shows recently to discuss new materials for energy including the Fred Friendly PBS series and the Ecopolis program on the Discovery Channel. He holds 11 current or pending U.S. patents.

# Dr. Gerould K. Young

**Director, Materials & Fabrication Technology**
**The Boeing Company**


## Atoms to Airplanes: Simulation, Testing and the Future of Design


### Abstract

Design cycles of aircraft require a great deal of time and investment to even get to the stage of building large engineering structures to be tested. Powerful analysis and simulation techniques such as computational fluid dynamics, finite element methods, and computer modeling are taking prominent roles to reduce this design cycle. The materials engineering community is now challenged to engage through ICME. This presentation reflects on design cycle changes over the last few decades and brings new insights on the ability to model and test at various size-scales – from the nano scale to large structures. Validation testing and advanced simulation are essential elements in the chain of events that are required to go from concept design, to the process development, to the manufacturing phase, and finally to product certification.


### Biography

Jerry leads the Materials and Fabrication Technology Organization for Boeing Research & Technology. This team of 600 engineers and scientists is developing next generation materials and manufacturing processes for existing and future Boeing products.

Prior to his current role, Jerry was the Director of Materials and Structures Technology, where he led Boeing's long-term R&D for materials, structural concepts and analysis tools. Jerry led three Boeing Joint Strike Fighter (JSF) technology programs for affordable titanium product forms casting, welding and forming and led Boeing's enterprise-wide development programs for Structural Analysis and Loads processes. He has worked on defense and commercial programs including B2, 777, F22 and JSF.

He holds a BS and MS in Mechanical Engineering from the University of Utah and is a graduate of the Advanced Management Program at University of Pennsylvania's Wharton Business School. He also holds four patents and has authored a number of technical papers.

# Professor Markus J. Buehler

**Laboratory for Atomistic and Molecular Mechanics (LAMM)**
**Esther and Harold E. Edgerton Associate Professor of Civil and Environmental Engineering, MIT**

## From Atoms to Structures, Turning Weakness to Strength

**Abstract**

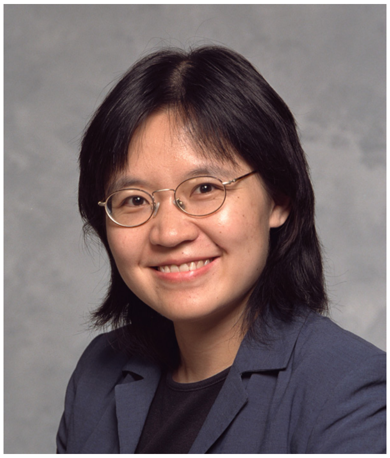
This talk will explain how materials in biology are synthesized, controlled and used for a variety of purposes—structural support, force generation, catalysis, or energy conversion—despite severe limitations in available energy, quality and quantity of building blocks. By incorporating concepts from chemistry, biology and engineering we describe how computational materials science has led the way in identifying the core principles that link the molecular structure of proteins at scales of nanometers to physiological scales at the level of tissues, organs, and organisms. We demonstrated that the chemical composition of biology's materials plays a minor role in achieving functional properties. Rather, the way components are connected at different length-scales defines what material properties can be achieved, how they can be altered to meet functional requirements, and how they fail in disease states. We have achieved this by using the world's fastest supercomputers to predict properties of complex materials from first principles, in a multiscale modeling approach that spans many orders of magnitude in scale. This method, combined with experimental studies, allows us to build virtual "in silico" material models that provide unseen insight into the workings of natural and synthetic materials from the bottom up.

We demonstrate this approach in a case study of spider silk, one of the strongest yet most flexible materials in Nature, despite being made out of some the simplest, most abundant and intrinsically weak proteins, including weak hydrogen bonding. We discovered that the great strength and flexibility of spider silk—exceeding that of steel and other engineered materials—can be explained by the material's unique structural makeup that involves multiple hierarchical levels from the nano- to the macroscale. These hierarchical levels span from the genetic information that defines the protein sequence to the structural scale of an entire spider web. Each level contributes to the overall properties, but the remarkable properties emerge because of the synergistic interaction across the scales where the sum is more than its parts. This concept explains how spider silk provides extreme functionality despite the simple basis in its makeup. By translating this insight gained from the study of natural materials such as spider silk to engineered materials such as carbon nanotube fibers, graphene composites or metal-polymer films, our research has resulted in an engineering paradigm that facilitates the design of sustainable materials starting from the molecular level, leading to the formation of hierarchical structures that span all scales from nano to macro, and leading to a merger of the concepts of structure and material.

We illustrate this concept by drawing an analogy to a seemingly far and distant field—music. Reminiscent of protein materials, the integrated use of structures at multiple scales is the key to provide superior functional properties despite limitations in available building blocks, a set of musical instruments such as piano, violin or cello. In music, tones are played at different pitch, accentuation or duration and then assembled into melodies. The collective interaction of melodies, played by different instruments and arranged in a particular way, eventually results in the powerful expression of a symphony. We discuss analogies with other biological materials such as collagen in bone, or intermediate filaments in cells, and present general approaches towards the design of adaptable, mutable and active materials. Our work enables a paradigm shift in the design of materials that exceed the properties of natural ones while being constructed with low energy use and from abundant and intrinsically poor material constituents.

## Biography

Markus J. Buehler is an Associate Professor in the Department of Civil and Environmental Engineering at the Massachusetts Institute of Technology, where he directs the Laboratory for Atomistic and Molecular Mechanics (LAMM). Buehler's research focuses on bottom-up modeling and simulation of structural and mechanical properties of biological, bioinspired and synthetic materials across multiple scales, with a specific focus on materials failure from a nanoscale and molecular perspective. Buehler has published more than 170 articles on computational materials science, nanotechnology and nanoscience, authored two monographs, and given several hundred invited, keynote and plenary talks. He was cited as one of the top engineers in the United States between the ages of 30-45 through invitation to the National Academy of Engineering-Frontiers in Engineering Symposium of the National Academy of Engineering. Buehler received the National Science Foundation CAREER award, the United States Air Force Young Investigator Award, the Navy Young Investigator Award, and the DARPA Young Faculty Award. In 2010 his work was recognized by the Presidential Early Career Award for Scientists and Engineers (PECASE), the highest honor bestowed by the United States government on outstanding scientists and engineers in the early stages of their careers. He also received the Harold E. Edgerton Faculty Achievement Award for exceptional distinction in teaching and in research or scholarship, the highest honor bestowed on young MIT faculty. Other major awards include the Thomas J.R. Hughes Young Investigator Award, the Sia Nemat-Nasser Medal, the Rossiter W. Raymond Memorial Award, the Stephen Brunauer Award, the Alfred Noble Prize, and the Leonardo da Vinci Award. Buehler serves as a member of the editorial board of several international journals including: BioNanoScience (as Editor-in-Chief), Roy. Soc. Interface, PLoS ONE, Int. J. Appl. Mech., Acta Mech. Sinica, J. Mech. Beh. Biomed. Mat., J. of Engrg. Mech., J. Nanomech. Micromech, and the J. Comp. and Theor. Nanosci. He is the founding chair of the Biomechanics Committee at the Engineering Mechanics Institute of ASCE, a member of the U.S. National Committee on Biomechanics, and participates actively in several committees at ASME.



# Dr. Yue Qi

**Staff Research Scientist**
**Chemical Sciences and Materials Processes Lab**
**General Motors R & D and Planning**

## Computational Materials Design - From Hard Coatings to Soft Membranes

### Abstract

Dramatic improvements have been made in computational techniques at different scales in the past few decades. Recently, by transferring parameters, equations, and insights obtained from smaller scale to larger scale, the combination and overlapping of these techniques bring material modeling into a truly multi-scale era. In this presentation, I will briefly overview how computational materials modeling were integrated with light weight and energy storage materials' research in automobile industries with examples. In one case, first principles calculations were integrated with cohesive zone and growth chemistry models to predict interface adhesion and growth stress of nano-crystalline diamond (NCD), in order to enable it as a tool coating for aluminum machining. In the second case, a coarse-graining approach was developed to obtain the morphologies of hydrated Nafion for fuel cells, where the network connectivity of hydrophilic domains strongly influences the proton conductivity and mechanical property of the membrane. In both cases, material modeling did not stop at explaining existing data or confirming experimental findings, but to make an experimentally testable prediction on how to optimize material structures and processing conditions before material synthesis.

### Biography

Dr. Yue Qi is a Staff Research Scientist working on computational materials sciences at Chemical Sciences and Materials Systems Lab, General Motors R&D Center. She completed her B.S. degrees on Materials Science and Computer Science at Tsinghua University in 1996. She received her PhD in Materials Science from California Institute of Technology in 2001 and joined GM R&D in the same year. In GM R&D, she has been using multi-scale modeling approach to solve problems related to energy materials for batteries and fuel cells, forming and machining of light weight alloys. Her recent research topic is on "integration of material properties into Li-ion battery failure modeling". She received GM Campbell awards (on research) for "Multi-scale Modeling of High-temperature Deformation in Aluminum" (2009), "Fundamentals of Interfacial Tribology"(2009), and "Advances in Nano-scale Plasticity" (2006). She was also the corecipient of 1999 Feynma Prize in Nanotechnology for Theoretical Work with Dr. T. Cagin and Prof. W. A. Goddard III (PhD advisor).

# Dr. Gerbrand Ceder

**R.P. Simmons Professor of Materials Science and Engineering**
**Department of Materials Science & Engineering, MIT**

## The "Materials Genome" Project: Accelerated and Large-Scale Materials Discovery through Computation

**Abstract**

The need for novel materials is the technological Achilles Heel of our strategy to address the energy and climate problem facing the world. The large-scale deployment of photovoltaics, photosynthesis, storage of electricity, thermoelectrics, or reversible fuel catalysis can not be realized with current materials technologies. The "Materials Genome" project, started at MIT, has as its objective to use high-throughput first principles computations on an unparalleled scale to discover new materials for energy technologies. Only computationally driven materials design can deal with the scale and urgency of the materials discovery problem. I will show how several key problems such as crystal structure prediction and accuracy limitations of standard Density Functional Theory methods have been overcome to perform reliable, large scale materials searching.

Successful examples will be shown of high-throughput calculations in the field of lithium batteries, several new materials that have been discovered and discuss developments in other fields. In addition, the public release version of the Materials Genome project which will be making large quantities of computed data freely available to the materials community will be shown.

**Biography**

Gerbrand Ceder is a Professor of Materials Science and Engineering at the Massachusetts Institute of Technology. He received an engineering degree from the University of Leuven, Belgium, and a Ph.D in Materials Science from the University of California at Berkeley in 1991 at which time he joined the MIT faculty. Dr. Ceder's research interests lie in the design of novel materials for energy generation and storage, including battery materials, hydrogen storage, thermoelectrics, electrodes for fuel cells and photovoltaics. He has worked for over 15 years in the Li-battery field, optimizing several new electrode materials and has regularly served as scientific advisor to companies and investors in this area. He has published over 270 scientific papers, and holds several U.S. patents. Dr. Ceder founded the Materials Genome Project, and his most recent scientific achievement has been the development of materials for ultra fast battery charging. He has received the MRS Gold Medal, the Battery Research Award from the Electrochemical Society for his work on understanding battery materials, the Career Award from the National Science Foundation, and the Robert Lansing Hardy Award from The Metals, Minerals and Materials Society. He is the founder of Computational Modeling Consultants and Pellion Technologies, and is currently an advisor to the Office of Strategic R&D Planning of the Korean Government. Dr. Ceder served as a member of the American Physical Society's study on Critical Elements for Energy Technologies.

# Professor Alfredo Alexander-Katz

**Department of Materials Science and Engineering, MIT**

## Soft Materials *in Silico:* Opening New Frontiers in Materials Science

**Abstract**

Soft materials are materials in which bonds between molecules are weak non-covalent bonds. Some natural examples are DNA, proteins, and biological membranes. These molecules have existed in our world for millions of years, and are the basis of life as we know it. Only during the last century, however, has mankind developed methods to synthesize polymers that resemble their biological counterparts. These polymeric soft materials, colloquially known as plastics, have revolutionized our world due to their outstanding properties that can be tailored for a wide variety of very specific needs, ranging from ultra high strength fibers to organic light emitting devices to biomedical devices. Soft materials thus represent a promising field of interdisciplinary research where computational material science can have a powerful impact by opening new frontiers in which previously unthinkable behaviors are now possible. In this talk I will highlight some of the "smart" emerging properties of different classes of soft systems studied in our research group. In particular, I will present our work in different systems in which responsive soft materials present interesting and promising phenomena that could have strong implications in future technologies. The systems that I will talk about range from directed block copolymer assembly to blood clotting and self-healing materials. In all cases, external fields in the form of confinement or flow dictate the state of the system, offering a new way to tailor the properties of these materials. Emphasis will be placed in the important role that simulations can provide in understanding and designing such systems.

**Biography**

Alfredo Alexander-Katz is an Assistant Professor in the Department of Materials Science and Engineering at the Massachusetts Institute of Technology. He earned his B. Sc. degree from the Universidad National Autonoma de Mexico (UNAM) and his Ph. D. from the University of California at Santa Barbara (UCSB), both in physics. Afterwards, he moved to the Technical University of Munich (Germany) as an NSF International Postdoctoral Fellow to study the dynamics of driven polymers. He later moved to the Ecole Superieure de Physique et Chimie Industrielle (Paris, France) as a CNRS postdoctoral researcher to study charged polymer solutions and their self-assembly with direct applications to fuel cells. His current interests lie in the realm of self-assembly and dynamics of biological soft-materials using a combination of analytical theory and simulations. He has won several distinctions including a NSF CAREER Award.

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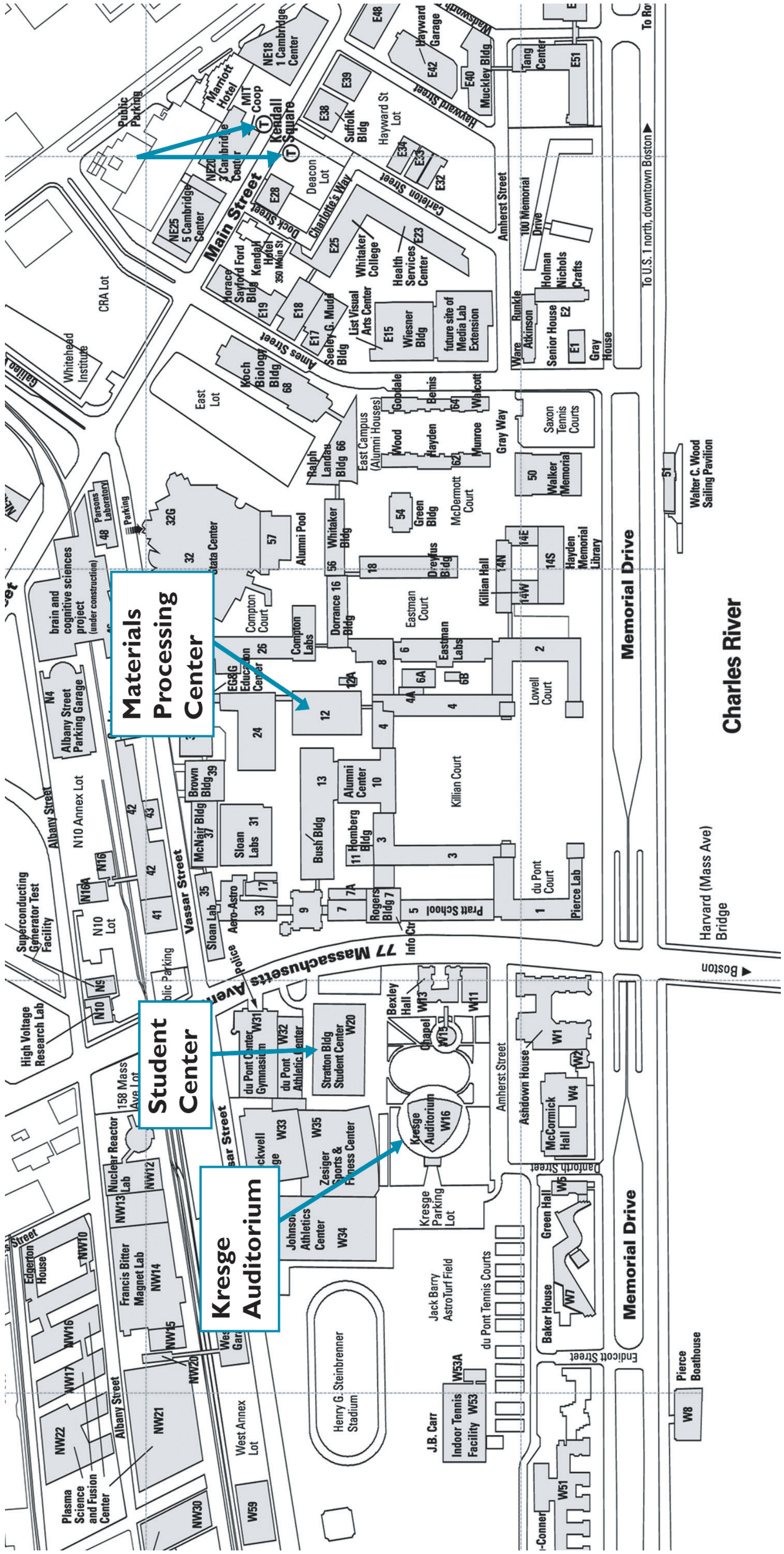
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Harvard (Mass Ave) Bridge
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Stratton Bldg Student Center W20
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mpc 30+ advancing materials research

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