MACHINE LEARNING IN MATERIALS RESEARCH

MATERIALS DAY

MRL
MIT
MATERIALS
RESEARCH
LABORATORY

Materials Resources

The Materials Research Laboratory (MRL) serves interdisciplinary groups of faculty, staff and students, supported by industry, foundations and government agencies to carry out fundamental engineering research on materials. Research topics include energy conversion and storage; quantum materials; spintronics; photonics; metals; integrated microsystems; materials sustainability; solid-state ionics; complex oxide electronic properties; biogels; and functional fibers.
https://mrl.mit.edu

The MRL MRSEC (formerly MIT MRSEC) at MIT is one of a nation-wide network of Materials Research Science and Engineering Centers sponsored by the National Science Foundation (NSF).
https://mitmrsec.mit.edu

The Crystal Physics and Electroceramics Laboratory is devoted to the modeling, processing, characterization and optimization of energy related devices (sensors, batteries, fuel cells, solar/photolysis cells) and the integration of sensor, actuator and photonic materials into microelectromechanical (MEMS) systems.
http://electroceramics.scripts.mit.edu/

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

The Communications Technology Roadmap (CTR) is a project under the Microphotonics Center Industry Consortium, and is a part of the 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 AIM Photonics Academy launched in 2016 as the education, workforce development, and roadmapping arm of AIM Photonics, one of 14 public-private manufacturing innovation institutes created as part of a federal initiative to revitalize American manufacturing. Currently, the AIM Photonics Academy administrative offices are hosted at MIT. The AIM Photonics Academy's mission is to educate the current and future workforce in integrated photonics – technologies that will lead to the next generation of faster and more power-efficient chips.
https://aimphotonics.academy/

The Skoltech Center for Electrochemical Energy Storage (CEES) is an inter-university/interdepartmental center with three major goals: development of advanced lithium ion and multivalent ion batteries, the development of rechargeable metal-air batteries, and the development of reversible low and elevated temperature fuel cells.
https://cees-www.mit.edu/

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

MATERIALS DAY AT MIT

Machine Learning in Materials Research

October 9, 2019

Recent advances in machine learning have increasingly been used in materials science research. Scientists and researchers are utilizing higher level computational methods to help leverage massive data streams of their findings for real world applications. The benefits of machine learning in materials science are vast and have completely changed the research arena. Speakers from industry as well as professors from MIT will be discussing their research, the specific challenges they have experienced and how using machine learning has led to new insights and breakthroughs.

The poster session immediately follows the symposium and showcases students research and it's applications. About sixty-five posters are presented each year, on a full range of research topics.

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Materials Day Agenda

8:00am	**Registration**
8:45 - 9:00am	**Welcome and Overview** Professor Carl V. Thompson Director, Materials Research Laboratory Professor, Department of Materials Science & Engineering, MIT
Session I:	
9:00 - 9:30am	**Keynote:** **Accelerating Materials Design and Discovery for Electric Vehicles** Dr. Brian Storey Director, Accelerated Materials Design & Discovery, TOYOTA Research Institute
9:30 - 10:00am	**Text and Data Mining for Material Synthesis** Associate Professor Elsa Olivetti Department of Materials Science & Engineering, MIT
10:00 - 10:30am	**Advanced Chemical Development Through Process Intensification, Automation, and Machine Learning** Professor Klavs F. Jensen Departments of Chemical Engineering and Materials Science & Engineering, MIT
10:30 - 11:00am	**BREAK**
11:00 - 12:00pm	**Poster Previews: 2 minute talks by selected poster presenters**
12:00 - 1:30pm	**LUNCH** Stratton Student Center, 3rd Floor Twenty Chimneys/Mezzanine Lounge (Building W20-306 & 307)

Agenda cont'd

Session II:

1:30 - 1:50pm	**Computing at MIT** Professor Asu Ozdaglar Deputy Dean of Academics and Electrical Engineering & Computer Science Department Head, MIT
1:50 - 2:20pm	**Machine Learning in Optics: From Spectrum Reconstruction to Metasurface Design** Associate Professor Juejun (JJ) Hu Department of Materials Science & Engineering, MIT
2:20 - 2:50pm	**Elastic Strain Engineering for Unprecedented Properties** Professor Ju Li Departments of Nuclear Science & Engineering and Materials Science and Engineering, MIT
2:50 - 3:20pm	**Learning Matter: Materials Design Through Atomistic Simulations and Machine Learning** Assistant Professor Rafael Gomez-Bombarelli Department of Materials Science & Engineering, MIT
3:20 - 3:30pm	**Session Wrap Up** Professor Carl V. Thompson Director, Materials Research Laboratory Professor, Department of Materials Science & Engineering, MIT
3:35 - 5:30pm	**Poster Session and Social** La Sala de Puerto Rico, 2nd Floor, Stratton Student Center (Building W20-202)
5:30pm	**Poster Awards**
5:45pm	**Adjourn**

Welcome and Overview

Biography: Professor Thompson received an S.B. in Materials Science and Engineering from MIT and a Ph.D. in Applied Physics from Harvard University. He joined the MIT faculty in 1983. He is the Director of MIT's Materials Research Laboratory and co-directs the Skoltech Center for Electrochemical Energy Storage. He previously directed the Materials Processing Center and co-chaired the Materials for Micro- and Nano-systems program of the Singapore-MIT Alliance for twelve years. He is also a past president and Fellow of the Materials Research Society. Professor Thompson's research interests include processing of thin films and nanostructures for applications in microelectronic, microelectromechanical and electrochemical systems. Current activities focus on development of thin film batteries for autonomous microsystems, the reliability of IC interconnects and GaN-based devices, and morphological stability of thin films and nano-scale structures.

Professor Carl V. Thompson
Director, Materials Research Laboratory
Stavros Salapatas Professor of Materials Science and Engineering
Department of Materials Science and Engineering, MIT

Accelerating Materials Design and Discovery for Electric Vehicles

Abstract: Developing truly emissions free transportation and mobility will remain one of society's grand challenges over the coming decades. The shift toward increased electrification is already presenting both new opportunities and new challenges for the auto industry. At TOYOTA Research Institute (TRI), we believe that a sustainable future will require new materials and our aim is to develop tools and capability to accelerate the pace of R&D on materials for battery and fuel cell electric vehicles. Given the scale of the problem, the strategy at TRI relies on close collaboration between industry and university research. This talk will discuss some ongoing collaborative projects at TRI as examples of how we believe we can start to make progress.

Biography: Brian Storey is Director of the Accelerated Materials Design and Discovery (AMDD) program at TOYOTA Research Institute. The goal of the AMDD program is to develop tools for accelerating the development of new energy materials for emissions free mobility. The AMDD program consists of an internal TRI research team as well as $10M/year of university sponsored research. In addition to his role at TOYOTA, Dr. Storey is a professor of mechanical engineering at Olin College. He has been on the faculty at Olin since 2000 and was one of the founding faculty members for this undergraduate, engineering focused college. Dr. Storey received his PhD from the University of California, Berkeley, M.S. from University of Illinois, and BS from the University of Texas, Austin - all in Mechanical Engineering.

Dr. Brian Storey
Director
Accelerated Materials Design & Discovery,
TOYOTA Research Institute

October 9, 2019

Text and Data Mining for Material Synthesis

Abstract: 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.

Biography: 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.

Elsa Olivetti
Associate Professor
Department of Materials Science and Engineering, MIT

Advanced Chemical Development Through Process Intensification, Automation and Machine Learning

Abstract: Process intensification via continuous operation combined with automated optimization and screening techniques offer opportunities for faster development and more efficient manufacture of diverse chemical products. This presentation starts with advances in process intensification and green chemistry achieved through micro-reaction technology and continuous multi-step synthesis (flow chemistry). Case studies include individual intensified reaction units as well as on-demand synthesis of common pharmaceuticals in a plug-and-play, manually reconfigurable, refrigerator-sized manufacturing platform. Next, advances in automated screening and optimization of chemical reactions are highlighted as methods to accelerate translation of laboratory discoveries to manufacturing. Examples include optimization of thermal and photo-chemical reactions in 15 microliter droplets with respect to continuous process conditions (temperature, time, concentrations…) and discrete process choices (catalysts, solvents, bases …). Finally, machine learning of chemical information is applied to computer aided chemical synthesis - the planning of reaction paths to a given molecular target from purchasable starting materials. With expert user input, the synthesis plans are converted into recipes that are executed by an automated modular continuous flow platform configured by a robotic arm, which sets up the required unit operations. Examples of automatic continuous syntheses of pharmaceutical compounds and libraries illustrate the promise of this combined approach of machine learning, reaction engineering, and robotics.

Biography: Klavs F. Jensen is the Warren K. Lewis Professor in Chemical Engineering and Materials Science and Engineering at MIT. From 2007- July 2015 he was the Head of the Department of Chemical Engineering. His research interests include on-demand multi-step synthesis, methods for automated synthesis, and machine learning techniques for chemical synthesis and interpreting large chemical data sets. He is a co-director of MIT's Pharma AI consortium that aims to bring machine learning technology into pharmaceutical discovery and development. Catalysis, chemical kinetics and transport phenomena are also topics of interest along with development of methods for predicting performance of reactive chemical systems. He chairs the Editorial Board for the new Royal Society of Chemistry, Journal Reaction Chemistry and Engineering. He serves on advisory boards to universities, companies, professional societies, and governments. He is the recipient of several awards, including the Allan P. Colburn, Charles C.M. Stine, R.H. Wilhelm, W.H. Walker, and Founders Awards of the American Institute of Chemical Engineers, and the inaugural IUPAC-ThalesNano Prize in Flow Chemistry. Professor Jensen is a member of the US National Academy of Sciences, the US National Academy of Engineering as well as the American Academy of Arts and Science. He is a Fellow of the American Association for the Advancement of Science (AAAS), and the American Institute of Chemical Engineers, and the Royal Society of Chemistry.

Klavs F. Jensen
Professor
Departments of Chemical Engineering and
Materials Science & Engineering, MIT

Computing at MIT

Abstract: Computing generally and computer science specifically have grown significantly in the last two decades. At MIT, a growing set of the faculty use computational methods in their research and more than 25% of our undergraduates major in computer science. The newly launched Schwarzman College of Computing (SCC) provides a critical opportunity to rethink how computing is taught across MIT and for bringing people together to foster research that combines computing with other disciplines. In this talk, I will talk about the computing landscape at MIT and present recommendations of the SCC Organizational Structures Working Group, which I have co-chaired with Professor Nelson Repenning from Sloan.

Biography: Asu Ozdaglar received her B.S. degree in electrical engineering from the Middle East Technical University, Ankara, Turkey, in 1996, and S.M. and Ph.D. degrees in electrical engineering and computer science from the Massachusetts Institute of Technology, Cambridge, in 1998 and 2003, respectively.

She is the Distinguished Professor of Engineering in the Electrical Engineering and Computer Science (EECS) Department at the Massachusetts Institute of Technology. She is also the department head of EECS. Her research expertise includes optimization theory, with emphasis on non-linear programming and convex analysis, game theory, with applications in communication, social, and economic networks, distributed optimization and control, and network analysis with special emphasis on contagious processes, systemic risk and dynamic control.

Professor Ozdaglar is the recipient of a Microsoft fellowship, the MIT Graduate Student Council Teaching award, the NSF Career award, the 2008 Donald P. Eckman award of the American Automatic Control Council, the Class of 1943 Career Development Chair, the inaugural Steven and Renee Innovation Fellowship, and the 2014 Spira teaching award. She served on the Board of Governors of the Control System Society in 2010 and was an associate editor for IEEE Transactions on Automatic Control. She was the inaugural area co-editor for the area entitled “Games, Information and Networks” in the journal Operations Research. She is the co-author of the book entitled “Convex Analysis and Optimization” (Athena Scientific, 2003).

Asu Ozdaglar
Professor and Department Head
Department of Electrical Engineering and Computer Science, MIT

Machine Learning in Optics: From Spectrum Reconstruction to Metasurface Design

Abstract: In this talk, we discuss two examples in our work where machine learning is applied to solving problems in optics. In the first example, we developed a machine learning regularization method to reconstruct optical spectra based on data measured from a chip-scale optical spectrometer. We show that the algorithm can significantly boost signal-to-noise ratio in optical spectrum acquisition, enabling two-fold enhanced spectral resolution compared to the classical Rayleigh criterion. In the second example, we introduce a generic deep neural network approach to vastly improve the throughput and accuracy of free-form optical metasurface design. Examples of neural networks capable of producing on-demand designs for meta-atoms, meta-optical filters, and reconfigurable metasurfaces are demonstrated.

Biography: Juejun (JJ) Hu received his B.S. degree from Tsinghua University, China, in 2004, and his Ph.D. degree from Massachusetts Institute of Technology, Cambridge, MA, USA, in 2009, both in materials science and engineering. He is currently the Merton C. Flemings Career Development Associate Professor in MIT's Department of Materials Science and Engineering. His primary research interest is enhanced photon-matter interactions in nanophotonic structures. Prior to joining MIT, he was an Assistant Professor at the University of Delaware from 2010 to 2014. Hu has authored and co-authored more than 70 refereed journal publications since 2006 and has been awarded six U.S. patents. He has been recognized with the National Science Foundation Faculty Early Career Development award, the Robert L. Coble Award from the American Ceramic Society, the Gerard J. Mangone Young Scholars Award, the University of Delaware College of Engineering Outstanding Junior Faculty Member, the University of Delaware Excellence in Teaching Award, among others.

Juejun Hu
Associate Professor
Department of Materials Science & Engineering, MIT

October 9, 2019

Elastic Strain Engineering for Unprecedented Properties

Abstract: Strain Engineering uses strain to guide the interactions of material structures with electrons, photons, etc. and control energy, mass and information flows. The success of Strained Silicon technology today harbingers what Strain Engineering may do for human civilization in the future, with potential breakthroughs in electronics, photonics, ferroics, superconductivity, catalysis, sensing, etc. In this talk I will give examples of exploiting the strain design space with machine learning. Homogenous and inhomogeneous elastic strain, bending, interlayer twist and slip lead to tunable, low-energy artificial atoms, artificial superlattices and pseudoheterostructures that can regulate quasiparticle motion. Strain also governs ferroelastic and band topology transitions in these materials. Lastly, we demonstrate production of kilogram-scale nanowires under large tensile elastic strain, that leads to improved superconductivity. By controlling the strain tensor and strain gradient statically or dynamically, one opens up a much larger parameter space -on par with alloying -for optimizing the functional properties of materials, which imparts a new meaning to Feynman's statement "There's Plenty of Room at the Bottom".

Biography: Ju Li is a Professor of Nuclear Science and Engineering and a Professor of Materials Science and Engineering at MIT. His group investigates the mechanical, electrochemical and transport behaviors of materials as well as novel means of energy storage and conversion. Ju is a recipient of the 2005 Presidential Early Career Award for Scientists and Engineers, the 2006 Materials Research Society Outstanding Young Investigator Award, and the TR35 award from Technological Review. Ju was elected Fellow of the American Physical Society in 2014 and a Fellow of the Materials Research Society in 2017. In 2014/2018 Thomson Reuters/Clarivate included him in the Highly Cited Researchers list in the Materials Science category. In 2016 Ju Li co-founded one of the MIT Energy Initiative (MITEI) Low-Carbon Energy Centers, the Center for Materials in Energy and Extreme Environments.

Ju Li
Professor
Departments of Nuclear Science & Engineering and
Materials Science & Engineering, MIT

Learning Matter: Materials Design Through Atomistic Simulations and Machine Learning

Abstract: Machine learning tools combined with theoretical simulations can effectively accelerate the design of novel materials. Data-driven approaches can access the information embedded in years of experiments, perform rapid optimization of high-dimensional experimental conditions and design parameters, increase the accuracy and speed of physics-based simulations, or design new molecules and crystals automatically. By deploying automated atomistic simulations (molecular dynamics, electronic structure) to create interpretable, bottom-up representations of materials, and by using those as inputs to machine learning models, we can build effective and accurate predictors. Here, we will describe recent results and ongoing work in using machine learning as the connector between multiple scales of simulation and experiment in materials design. These include (i) high-throughput screening of molecular materials such as organic light emitting-diodes, small molecule battery electrolytes, or photovoltaics using electronic structure simulations; (ii) inverse design tools based on deep generative models for automatic chemical discovery; (iii) automated learning of all-atom and coarse-grained potentials for discovery of soft materials like ion-conducting polymers; (iv) graph-based representations that accurately predict and rationalize polymorphism in nanoporous zeolite materials.

Biography: Rafael (Rafa) Gomez-Bombarelli received his BSc, MSc (2006) and PhD (2011) in Chemistry from Universidad de Salamanca (Spain). After postdoctoral work at Heriot-Watt University (Edinburg, UK 2012-2014) and Harvard's Department of Chemistry and Chemical Biology (2014-2016), Rafa co-founded Calculario, a materials discovery start-up and joined Kyulux North America Inc., an OLED start-up focused in thermally-assisted delayed fluorescence materials for display. Since January 2018 Rafa is an Assistant Professor at MIT- DMSE. There, he leads a 10-people group working at the interface between deep learning and atomistic simulations for materials design, with a strong focus on molecular and nanoporous materials, inverse design and dimensionality reduction, and supramolecular recognition. He was recently awarded the Google Faculty Research Award (2019).

Rafael Gomez-Bombarelli
Assistant Professor
Department of Materials Science & Engineering, MIT

Kresge Auditorium - W16
Stratton Student Center - W20

Dates for future Materials Day events:

October 14, 2020

October 20, 2021

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