MIT Industrial Liaison Program Faculty Knowledgebase Report

Computationally-Assisted Materials Discovery

April 10, 2025 10:00 am - 12:00 pm

10:00 AM	Welcome and Opening Remarks Jewan Bae Program Director, MIT Corporate Relations

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Program Director, MIT Corporate Relations

Jewan John Bae comes to MIT Corporate Relations with more than 20 years of experience in the specialty chemicals and construction industries. He facilitates fruitful relationships between MIT and the industry, engaging with executive level managers to understand their business challenges and match them with resources within the MIT innovation ecosystem to help meet their business objectives.

Bae's areas of expertise include new product commercialization stage gate process, portfolio management & resource planning, and strategic planning. He has held various business leadership positions at W.R. Grace & Co., the manufacturer of high-performance specialty chemicals and materials, including Director of Strategic Planning & Process, Director of Sales in the Americas, and Global Strategic Marketing Director. Bae is a recipient of the US Army Commendation Medal in 1986.

10:02 AM

Computer-Aided Design of Small Molecules and Procedures to Synthesize Them
Connor W. Coley

Class of 1957 Career Development Professor and Assistant Professor,
MIT Chemical Engineering and MIT Electrical Engineering and Computer Science

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MIT Chemical Engineering and MIT Electrical Engineering and Computer Science

Connor W. Coley is the Class of 1957 Career Development Professor and an Assistant Professor at MIT in the Department of Chemical Engineering and the Department of Electrical Engineering and Computer Science. He received his B.S. and Ph.D. in Chemical Engineering from Caltech and MIT, respectively, and did his postdoctoral training at the Broad Institute. His research group at MIT works at the interface of chemistry and data science to develop models that understand how molecules behave, interact, and react and use that knowledge to engineer new ones, with an emphasis on therapeutic discovery. Connor is a recipient of C&EN's "Talented Twelve" award, Forbes Magazine's "30 Under 30" for Healthcare, Technology Review's 35 Innovators Under 35, the NSF CAREER award, the ACS COMP OpenEye Outstanding Junior Faculty Award, the Bayer Early Excellence in Science Award, the 3M NTFA, and was named a Schmidt AI2050 Early Career Fellow and a 2023 Samsung AI Researcher of the Year.

Generative molecular design seeks to propose novel molecular structures that may surpass what is available in enumerated virtual libraries. While enumerated libraries are large, the enormity of chemical spaces means that there are ample opportunities for "creativity" in molecular design. Often, this creativity leads to ideas of molecules that are difficult to produce experimentally--a crucial bottleneck for discovery. I will describe a generative framework that mitigates lack of synthesizable as a major failure mode of design. Our model ensures that every generated molecule has a viable synthetic pathway, enabling the design of analogs and optimization of molecular properties while maintaining synthetic feasibility. By providing effective and controllable navigation within synthesizable chemical space, we can provide actionable suggestions of new small organic molecules across a range of fields, including drug development and materials science.

10:32 AM

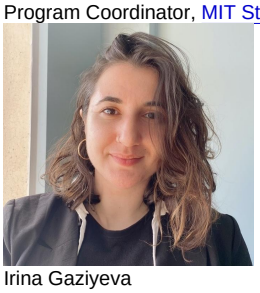
Computational Assessment of the Stability of Inorganic Solid Materials

Rodrigo Freitas

Assessment of material stability is a major bottleneck in the discovery of inorganic solid materials – such as green metallic alloys, semiconductors in microelectronics, ceramics in fuel cells, and superconductors for fusion energy. A reliable approach for the computational evaluation of stability will accelerate the discovery of novel materials by avoiding searches of synthesis pathways for unsynthesizable (i.e., unstable) materials. In this webinar, I will introduce an approach that integrates a nascent generation of computational techniques that blend machine learning and physics-based methods to eliminate extrapolations and approximations that limit the accuracy and physical fidelity of computational stability predictions. The result is a computationally efficient methodology for on-demand access to accurate stability predictions that is readily applicable in conjunction with high-throughput experimentation and (semi-) autonomous laboratories.

11:02 AM

MIT Startup Exchange
Irina Gaziyeva
Program Coordinator, MIT Startup Exchange



Irina Gaziyeva
Program Coordinator
MIT Startup Exchange

Irina Gaziyeva comes to Corporate Relations from the Mechanical Engineering Department at MIT where she worked 10 years as Administrative Assistant where she has supported four senior faculty members and their research groups (20-25 graduate students). Since 2018, Irina has acted as program coordinator, teaming-up with the program manager and program faculty lead for the MechE Alliance program. She has facilitated 45+ virtual seminars, workshops, and mentoring events in this informal role. Irina has also actively connected members of the MechE community to support student career development, mentorship, and networking opportunities with MIT alumni and industry. Before MIT, Irina held positions as Administrative Assistant and Member Representative at Brookline Dental and Tufts Health plan, respectively. Irina has also been a Community Organizer in Worcester, MA.

Irina earned her B.A., Management (with Innovation & Entrepreneurship track) at Clark University in Worcester, and her M.S., Program and Project Management from Brandeis University in Waltham. She has received many awards at MIT for outstanding service, and she has extensive community volunteer work to her credit.

Jason Sebastian

Jacob Grose

Alexander O'Brien

Fred Liu

11:30 AM

Towards AI-Driven Closed-Loop Materials Discovery
Rafael Gomez-Bombarelli

Paul M. Cook Career Development Professor,
Associate Professor, MIT Department of Materials Science and Engineering

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Professor Gómez-Bombarelli received his BS, MS, and PhD in chemistry from the University of Salamanca in Spain, followed by postdoctoral work at Heriot-Watt University in Scotland. As a postdoc at the Aspuru-Guzik lab at Harvard University he worked on high-throughput virtual screening for organic light-emitting diode (OLED) and battery electrolytes. He entered industry in 2016 as a senior researcher at Japanese technology company Kyulux, applying Harvard-licensed technology to build commercial OLED products. He joined the DMSE faculty in 2018.

Professor Gómez-Bombarelli's work has been featured in publications such as *MIT Technology Review* and the *Wall Street Journal*. He is co-founder of Calculario, a materials discovery company that uses quantum chemistry and machine learning to target advanced materials in a range of high-value markets.

View full bio

Innovations in areas like energy and sustainability, healthcare, or semiconductors are dependent on the discovery of new high-performance materials. The success of AI in day-to-day tasks like processing natural language or images, has seeded rapid and impactful developments in AI for science in the last years, from supervised learning to generative models.

Two key factors limiting the impact of AI in materials science are the lack of datasets in the scale of other applications, and the need to translate digital innovations into tangible materials.

Here we will describe how high-throughput physics-based simulations can produce large enough datasets to power deep learning models applied to materials discovery. In parallel, data mining the patent and scientific literature can capture domain knowledge to jump-start deep learning models. Lastly, closed-loop laboratory validation can validate computational predictions and further extend datasets to the needed scale.

We will report recent work of AI-powered, laboratory-validated, materials discovery in the areas of heterogeneous catalysis (synthesis and reactivity of zeolite catalysts, surface structure and activity of transition metal oxides), battery materials (polymer electrolytes), sustainable plastics (degradable thermosets), etc

11:58 AM

Closing Remarks
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12:00 PM

Adjournment