MIT Industrial Liaison Program Faculty Knowledgebase Report

Application of AI to Manufacturing Sustainability

April 28, 2022 12:00 pm - 2:00 pm

11:00 AM - 11:05 AM

Welcome & Introduction
Peter Lohse
Program Director, MIT Corporate Relations

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Dr. Peter Lohse joined the Office of Corporate Relations (OCR) in October 2018 as Program Director.

Lohse comes to OCR with deep and broad knowledge and expertise in the pharma, biotech, and other life sciences-driven industries including agro, nutrition, chemical, and consumer products. As a scientist and entrepreneur, he has an extensive background developing business and managing partnerships with large corporations, early-stage companies, academia, and non-profit organizations. Most recently, Lohse was V.P, Operations and Business Development for InnovaTID Pharmaceuticals in Cambridge. Before that, he was a Strategy Consultant for Eutropics Pharmaceuticals, an emerging biotech company in Cambridge.

Prior to this, Dr. Lohse was Director, Scientific Operations & Innovation Program Director for Eli-Lilly's open innovation platform, InnoCentive, Inc. in Waltham. Earlier in his career, he held positions with increasing responsibility at ArQule of Woburn, Phylos in Lexington, and Novartis Pharma in Switzerland.

Lohse earned his M.S., Chemistry & Applied Sciences and his Ph.D., Organic Chemistry at Federal institute of Technology (ETH) in Switzerland. He earned his M.B.A., Strategy, Finance, Marketing as a Sloan Fellow at MIT. He also held the position Research Fellow, Molecular Biology at Harvard Medical School - Massachusetts General Hospital, Boston (with Professor J. Szostak, Nobel Prize 2009), This was a Swiss National Science Foundation Postdoctoral Fellowship -- In vitro selection of functional RNAs.

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11:05 AM - 11:35 AM

AI & ML for Predicting Chemical Reaction Systems and Solvation

William H. Green
Hoyt Hottel Professor in Chemical Engineering, MIT Department of Chemical Engineering

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Hoyt Hottel Professor in Chemical Engineering
MIT Department of Chemical Engineering

William Green is the Hoyt C. Hottel Professor of Chemical Engineering. He is a world leader in computer-aided chemical kinetic modeling, and leads a team of 20 researchers focusing on reaction kinetics, quantum chemistry, numerical methods, and fuel chemistry. In addition to his extensive work on kinetic modeling and combustion, oxidation, and pyrolysis chemistry, he has performed techno-economic assessments of proposed fuel and vehicle changes and biofuel production options, and he has published several papers on spectroscopy, numerical methods, and on applications of machine-learning to chemical problems. He has also addressed a variety of industrial engineering problems involving fuels, catalysis, and emissions. His work has been presented in more than 300 articles, which have cumulatively been cited more than 14,000 times. His research has been honored with several major awards including the AIChE 2019 Wilhelm Award in Reaction Engineering. He was named a Fellow of the Combustion Institute in 2018, and a Fellow of the American Association for the Advancement of Science in 2016. Prof. Green received his BA in Chemistry (with Highest Honors) from Swarthmore College in 1983, and his PhD in Physical Chemistry from the University of California, Berkeley in 1988. After postdoctoral research at Cambridge University and the University of Pennsylvania, he was a principal investigator at Exxon's Corporate Research Laboratory for six years before joining the MIT faculty in 1997. He chaired the sessions on Combustion at the AIChE National Meetings for a decade, and played a leadership role in the DOE's Combustion Energy Frontier Research Center. He convened the 7th International Conference on Chemical Kinetics at MIT in 2011. He served as Executive Officer of the MIT Department of Chemical Engineering from 2012-2015, and was the Editor of the *International Journal of Chemical Kinetics* from 2008-2013. He has been granted several patents and is a co-founder of the start-up company Thiozen which is commercializing one of them, a method for converting H2S into H2 with minimal CO2 emissions.

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There are a vast number of molecules and reaction networks. So although millions of chemical systems have been studied – so many that it is impossible for any human to begin to appreciate all the chemistry that is known – many more chemical systems have never even been considered. Today some chemical quantities are best obtained by (rather complicated) first-principles calculations, others are best obtained by (often complicated) experiments, and some quantities remain quite difficult to determine. Here we present several different Artificial Intelligence and Machine Learning approaches we have employed to predict the behavior of new chemical systems. Several AI/ML methods for combining experimental data and first principles equations/calculations to obtain more reliable predictions are presented. Some of these AI/ML prediction methods are very successful, and helpful for designing chemical processes.

11:35 AM - 12:05 PM

Computational Design of Nanoporous Catalysts for sustainable Transformations -- Video time stamp starts at: 34:38
Rafael Gomez-Bombarelli

Jeffrey Cheah Career Development Chair,
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.

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Zeolites are nanoporous aluminosilicate materials with broad applications in catalysis and separations. They are extremely versatile because of their topological diversity, with over 250 known polymorphs and thousands more predicted to be possible. However, managing polymorphism and phase competition in zeolite synthesis is a high-dimensional combinatorial problem that typically requires intensive trial and error in the lab.

High-throughput computational tools, built on a combination of theoretical and data-driven approaches and validated retroactively against computer-extracted literature, can produce insights and quantitative predictions for controlling these phases. In the case of solid-state inter zeolite transformations, we have found that graph-similarity between frameworks explains all hitherto known cases of diffusionless transformations and intergrowth and new ones reported thereafter.

In the case of templated zeolite crystallization, we propose new affinity and selectivity metrics between zeolite and organic structure-directing agents (OSDAs) that rationalize framework competition. Based on these principles and using over 1 million OSDA-zeolite simulations, we realize novel simple OSDAs the selectively synthesize AEI and CHA zeolites that outperform state-of-the-art methanol-to-olefin (MTO) catalysts multiple fold. Lastly, we predict and demonstrate an aluminosilicate CHA/AEI intergrowth using a single bi-selective OSDA.

12:05 PM - 12:35 PM

Bio-Inspired Material Intelligence -- Video time stamp starts at: 1:04:06
Markus J. Buehler

Jerry McAfee Professor of Engineering, MIT Department of Civil and Environmental Engineering and MIT Department of Mechanical Engineering

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Dr. Markus J. Buehler, Jerry McAfee Professor of Engineering at MIT, is a leading researcher in computational modeling across domains, from materials to biology to physics. Markus' expertise bridges AI to multi scale materials modeling. He recently co-developed a method that uses artificial intelligence to generate new protein designs with specific strengths, mimicking natural materials like silk. This approach, which uses computer simulations for testing, allows the creation of proteins with desired mechanical properties, such as strength and flexibility, beyond what is naturally available. Markus earned a Ph.D. at the Max Planck Institute for Metals Research at the University of Stuttgart and held post-doctoral appointments at both Caltech and MIT. Buehler has received many awards, including the Feynman Prize, the Drucker Medal, and the Washington Award. He is a member of the National Academy of Engineering.

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Digital materials are designed through an integrated approach of large-scale computational modeling, material informatics, and artificial intelligence/machine learning to optimize and leverage novel smart material manufacturing. Through the use of nanotechnology and additive manufacturing, and bio-inspired methods, we can now mimic and improve upon natural processes by which materials evolve, are manufactured, and how they meet changing functional needs. In this talk we show how we fabricate innovative materials from the molecular scale upwards, with built-in bio-inspired intelligence and novel properties, while sourced from sustainable resources, and breaking the barrier between living and non-living systems. This integrated materiomic approach is revolutionizing the way we design and use materials, and has the potential to impact many industries, as we harness data-driven modeling and manufacturing across domains and applications.

12:35 PM - 12:55 PM

A New World of Materials -- Video time stamp starts at: 1:44:41

Tonio Buonassisi
Co-Founder & Scientific Advisor, and MIT Professor of Mechanical Engineering
Xinterra

Xinterra pioneered the combined use of high throughput experimentation and artificial intelligence applied to materials, seeking efficient approaches to overcome slowness, high costs and overall limitation to innovation imposed by traditional materials R&D processes. Buonassisi will discuss Xinterra's combined use of high throughput experimentation and artificial intelligence applied to materals.