HAJIM SCHOOL OF ENGINEERING & APPLIED SCIENCES
UNIVERSITY of ROCHESTER

The Department of Chemical Engineering Presents:

Kwang-Yu & Lee-Chien Wang Fellowship Lecture

Mehrad Ansari, PhD Candidate
Renjie Liu, PhD Candidate
&
Prof. Heather Kulik, MIT

September 28, 2022
Poster Session 3—5 PM
Atrium, Goergen Hall
Talks beginning at 4 PM
101 Goergen Hall

Mehrad Ansari, Wang Fellowship Winner

Rescuing Physics-based Models with Maximum Entropy Reweighting

Mathematical modeling of disease outbreaks can infer the future trajectory of an epidemic, allowing for making more informed policy decisions. Another task is inferring the origin of a disease, which is relatively difficult with current mathematical models. Such frameworks, across varying levels of complexity, are typically sensitive to input data on epidemic parameters, case counts, and mortality rates, which are generally noisy and incomplete. To alleviate these limitations, we propose a maximum entropy framework that fits epidemiological models, provides calibrated infection origin probabilities, and is robust to noise due to a prior belief model. Entropy in information theory is directly analogous to the entropy in statistical thermodynamics. We evaluate the performance of our model by predicting future disease trajectories based on simulated epidemiological data in synthetic graph networks and the real mobility network of New York State. Indeed, despite the prevalent belief on the feasibility of contact-tracing being limited to the initial stages of an outbreak, we report the possibility of reconstructing early disease dynamics, including the epidemic seed, at advanced stages.

Mehrad Ansari is a PhD candidate of Chemical Engineering at the University of Rochester. Mehrad received his B.Sc. in Chemical Engineering from University of Tehran, Iran. He obtained his M.Sc. in Environmental Engineering at Missouri S&T. At the White Lab, Mehrad's PhD research is focused on physics-informed machine learning and simulation-based inference applied to different settings such as fluid dynamics, disease modeling and bioinformatics. His research interests involve developing a better connection between real-world experimental data and simulation space.

Renjie Liu, Wang Fellowship Winner

CO_2 Upgrading to Value-added Chemicals and Fuels

The CO_2 concentration in atmosphere monotonically increases starting from industrial revolution. Researchers have developed novel technologies for carbon capture to mitigate the global warming. The captured CO_2 can be used as a low-cost feedstock for CO_2 hydrogenation, transforming CO_2 into value-added chemicals and fuels and making the entire process carbon-neutral.
Recently, we have established several transition-metal based catalysts to promote the hydrogenation of CO and CO_2, producing light olefins and jet fuels. The secondary cracking behavior introduced by dual-functional catalysts have been applied to make light olefins and narrow down the product distribution. Additionally, a class of single atom catalysts have been studied to produce jet fuels at mild temperatures onboard a nuclear-powered aircraft carrier. The research can decrease dependence on fossil fuels as part of a future circular carbon economy.

Renjie Liu received his master's degree from the University of Rochester in 2019 and is currently pursuing his Ph.D. His research focuses on dual-functional catalysts for CO_2 and CO conversion to plastics, chemicals and fuels.

Molecular design blueprints: material and catalysts from new simulation and machine learning tools

Heather J. Kulik, PhD

Massachusetts Institute of Technology

I will discuss our efforts to use machine learning (ML) to accelerate the computational tailoring and design of transition metal complexes and metal-organic framework (MOF) materials for outstanding challenges in resource utilization, including catalysis, separations, and energy storage. One limitation in a challenging materials space such as open shell, 3d transition metal chemistry is that ML models and ML-accelerated high-throughput screening traditionally rely on density functional theory (DFT) for data generation, but DFT is both computationally demanding and prone to errors that limit its accuracy in predicting new materials. I will describe three ways we've overcome these limitations: i) through efficient global optimization to minimize the numbers of calculations carried out to obtain design rules in weeks instead of decades while satisfying multiple objectives; ii) through machine-learned consensus from a family of dozens of functionals to more robustly uncover new materials; and iii) by the use of natural language processing to extract, learn, and directly predict experimental measures of stability on heterogeneous MOF materials.

Professor Heather J. Kulik is a tenured Associate Professor in the Department of Chemical Engineering at MIT. She received her B.E. in Chemical Engineering from the Cooper Union in 2004 and her Ph.D. from the Department of Materials Science and Engineering at MIT in 2009. She completed postdoctoral training at Lawrence Livermore and Stanford, prior to joining MIT as a faculty member in November 2013. Her research has been recognized by an Office of Naval Research Young Investigator Award, DARPA Young Faculty Award and Director's fellowship, NSF CAREER Award, and a Sloan Fellowship in chemistry, among others.

Kwang-Yu Wang '70 (MS), '73 (PHD)

Wang began his career as a glass technologist in a major glass-bottle making plant in Singapore, subsequently becoming its general manager. In 1982, he founded Glastech, a Singapore-based glassware manufacturer and exporter. He ventured into property development, founding Glastech Investment in the early 1990s, as well as hospitality services, founding Wangz Hospitality Management Company in the 2000s. Wang has extensive industrial and business experience, and has been involved in the marketing of both industrial and consumer products in Singapore, Malaysia, South Africa, and the Middle East.

Spirit. The intent of the Kwang-Yu and Lee-Chien Wang Fellowship is to support excellence in Chemical Engineering research at the graduate level. The fellowship targets research in UR ChE's strategic focus areas: (i) sustainable energy and sustainable process engineering, (ii) optical, photonic and electronic materials, and (iii) computational driven materials discovery.

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Chemical Engineering (ChE) at the University of Rochester (UR) embodies high quality, multidisciplinary research and education in an idea-rich environment derived from its diverse faculty, staff, and students.

Tradition: founded in 1915, it is one of the first chemical engineering departments in the world. Virtually all ChE students learn from textbooks written by our professors and alumni.

Expertise: materials, applied electrochemistry, biotechnology, catalysts and computation.

Collaboration: research across campus with partners in Chemistry, Materials Science, Physics, Mechanical Engineering, Computer Science, Biomedical Engineering, the Laboratory for Laser Energetics and the School of Medicine and Dentistry.

Prominence: leaders include Professor Emeritus Ching Tang as father of the impactful OLED & late Professor Gouq-Jen (Gene) Su with landmark papers on applied thermodynamics.

Distinction: two NSF Faculty Early Career Development (CAREER) Awards (2018-2019), an 'Oscar of Invention' Award, and the 2019 Kyoto Prize.

Ranking: between 8 and 28 of ChE doctoral programs in the United States by the last National Research Council ranking report in 2010.