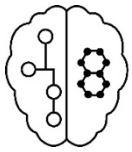

MMLI Dream and Visioning Workshop

The NSF-funded Molecule Maker Lab Institute (MMLI) is an interdisciplinary initiative, through which leaders in AI and organic synthesis (both chemical and biological) will intensively collaborate to create frontier AI tools, dynamic open access databases, and fast and broadly accessible small molecule manufacturing and discovery platforms.

Purpose

The goal of the "Molecule Maker Lab Institute (MMLI) Dream and Visioning Workshop" is to learn from thought leaders in using AI for organic synthesis and catalyst design and draw out what grand challenges remain. Leveraging the experience and vision provided by the invited speakers, group discussions in breakout sessions will then focus on how MMLI researchers can work toward making dreams a reality.

Date

Session 1: October 6, 2020, between 8:30 a.m – 1:00 p.m. (CT)
Session 2: October 14, 2020, between 1:00 p.m. – 5:30 p.m. (CT)

Audience

The MMLI Dream and Visioning Workshop presentations are open to both MMLI members and the broader research community interested in applying AI to synthesis and catalyst design.
*Space is limited to 300 attendees.
The Breakout Session at the end of each day is targeted to the MMLI members and participation is by invitation only.

Format

Speakers will be given 20 minutes with 10-12 minutes to describe their research and 8-10 minutes to talk about where the knowledge gaps exist and what their dream five-year deliverable would be from the Institute. Following each talk, participants can ask questions and the group will discuss the ideas presented. At the end of each day the group will break into ~4 teams (~10 people each) to discuss how the "dreams" from the presentations can shape the research goals for the MMLI.

Important Information for the Participants:

- This virtual workshop will be via Zoom.
- Participants must register to attend the workshop. **Zoom will deny your access to the workshop if you are not registered.**
- **Please note that Zoom will grant access to the workshop based on the e-mail address you provided during registration.** Thus, when logging in to the workshop, you have to use the same e-mail address you provided during registration.
- Upon approval by the host, participants will receive a confirmation e-mail with the information on how to join the workshop, including the meeting ID and password.
- Participants must use the Zoom desktop client, mobile app or telephone to join the meeting. Participants will NOT be able to join using the web client.
- There will be a separate Zoom meeting ID and password for Session 1 and Session 2.
- For workshop related questions, please contact Ipek Tasan at tasan2@illinois.edu

Agenda

Day 1: October 6, 2020

Start time: 8:30 a.m. (CT)
End time: 1:00 p.m. (CT)

8:00 a.m. – 8:30 a.m.	Meeting room opens

Opening Remarks

8:30 a.m. – 8:40 a.m.	Huimin Zhao, MMLI Director
8:40 a.m. – 8:45 a.m.	Laura Anderson, NSF

Session 1: AI-driven Synthesis Planning

8:45 a.m. – 1:00 p.m.	**Session Chair: Costas Maranas, MMLI**
8:45 a.m. – 9:00 a.m.	Jian Peng, MMLI Thrust 1 Leader
9:00 a.m. – 9:10 a.m.	Q&A
9:10 a.m. – 9:30 a.m.	Bartosz A. Grzybowski, Institute for Basic Science
9:30 a.m. – 9:45 a.m.	Q&A
9:45 a.m. – 9:55 a.m.	Break
9:55 a.m. – 10:15 a.m.	Keith E. J. Tyo, Northwestern University
10:15 a.m. – 10:30 a.m.	Q&A
10:30 a.m. – 10:50 a.m.	Connor W. Coley, Massachusetts Institute of Technology
10:50 a.m. – 11:05 a.m.	Q&A
11:05 a.m. – 11:25 a.m.	Eleni Litsa, Rice University
11:25 a.m. – 11:40 a.m.	Q&A
11:40 a.m. – 11:50 a.m.	Break

Breakout Session (by Invitation Only)

11:50 a.m.– 12:40 p.m.	Breakout Session
12:40 p.m. – 1:00 p.m.	Report out/Wrap up

Day 2: October 14, 2020

Start time: 1:00 p.m. (CT)
End time: 5:30 p.m. (CT)

12:30 p.m. – 1:00 p.m.	Meeting room opens

Session 2: AI-driven Catalyst Design

1:00 p.m. – 5:30 p.m.	**Session Chair: Christina White, MMLI**
1:00 p.m. – 1:15 p.m.	Scott E. Denmark, MMLI Thrust 2 Leader
1:15 p.m. – 1:20 p.m.	Q&A
1:20 p.m. – 1:40 p.m.	Leroy (Lee) Cronin, University of Glasgow
1:40 p.m. – 1:55 p.m.	Q&A
1:55 p.m. – 2:15 p.m.	Matthew S. Sigman, University of Utah
2:15 p.m. – 2:30 p.m.	Q&A
2:30 p.m. – 2:40 p.m.	Break
2:40 p.m. – 3:00 p.m.	Spencer D. Dreher, Merck
3:00 p.m. – 3:15 p.m.	Q&A
3:15 p.m. – 3:35 p.m.	Alán Aspuru-Guzik, University of Toronto
3:35 p.m. – 3:50 p.m.	Q&A
3:50 p.m. – 4:00 p.m.	Break

Breakout Session (by Invitation Only)

4:00 p.m. – 5:00 p.m.	Breakout Session
5:00 p.m. – 5:30 p.m.	Report out/ Wrap up/Thanks

Invited Speakers

Alán Aspuru-Guzik

https://www.matter.toronto.edu/

Alán Aspuru-Guzik is a professor of Chemistry and Computer Science at the University of Toronto. The mission of his research group is to accelerate the discovery of new chemicals and materials that are useful to society by means of new technologies such as quantum computing, machine learning, and automation.

Connor W. Coley

https://coley.mit.edu/

Connor W. Coley is an Assistant Professor in MIT's Department of Chemical Engineering and his research group develop platform technologies and workflows with relevance to drug discovery, chemical synthesis, and materials science.

Leroy (Lee) Cronin

http://www.chem.gla.ac.uk/cronin/

Leroy (Lee) Cronin is the Regius Professor of Chemistry at the University of Glasgow. Research in the Cronin Group is motivated by the fascination for complex chemical systems, and the desire to construct complex functional molecular architectures that are not based on biologically derived building blocks.

Spencer D. Dreher

Spencer D. Dreher is the lead scientist in Merck's Chemistry Capabilities and Screening group in Discovery Chemistry. The aim of his team is to accelerate the design, make and test cycle in small-molecule drug discovery to deliver results faster.

Bartosz A. Grzybowski

http://grzybowski-group.net/people/bartosz.asp

Bartosz A. Grzybowski is the Group Leader of the Center for Soft and Living Matter at the Institute for Basic Science (IBS) and Professor of Chemistry at the Ulsan National Institute of Science & Technology. He is also the co-founder of Allchemy. His current research interests include non-equilibrium self-assembly, reaction-diffusion phenomena, "thinking" materials, chemical networks and systems, theory of organic synthesis, and applications of AI to chemistry.

Eleni Litsa

http://www.kavrakilab.org/

Eleni Litsa is a graduate student in the laboratory of Lydia Kavraki at the Rice University. Kavraki group focuses on development of novel computational methodologies for Robotics & AI and Biomedicine. As part of her studies in the Kavraki group, Eleni Litsa recently developed a method for predicting drug metabolites using techniques from neural machine translation.

Matthew S. Sigman

https://chem.utah.edu/directory/sigm

Matthew S. Sigman is the Professor of chemistry at the University of Utah. His group is focused on the discovery of new practical catalytic reactions with broad substrate scope, excellent chemoselectivity, and high stereoselectivity to access novel medicinally relevant architectures.

Keith E. J. Tyo

https://tyolab.northwestern.edu/

Keith E. J. Tyo is an Associate Professor of Chemical and Biological Engineering at the Northwestern University. His group studies methods to modify existing environmental detection sensors in yeast and modify them to detect new analytes. His group also investigates ways microbes modify their metabolic networks and use these modifications to increase production of a given metabolite.