

MOLECULE  
MAKER LAB  
INSTITUTE



## Molecule Maker Lab Institute (MMLI)

Many of the greatest challenges facing society today likely have molecular solutions that await discovery.

The MMLI is an interdisciplinary initiative with leaders in AI and organic synthesis collaborating to create frontier AI tools, dynamic open access databases, and fast and broadly accessible small molecule manufacturing and discovery platforms.

# OUR EXPERTISE

The MMLI has brought together a world-leading team of researchers with highly complementary expertise in AI and ML, chemical and biological catalysis, enzyme engineering, materials synthesis and characterization, and outreach and workforce development.

## Technical Capabilities:

- Advanced ML algorithms for catalyst discovery, molecular function prediction, and process optimization
- Advanced text and image mining tools for data curation and knowledge extraction
- Advanced synthesis planning tools
- Dynamic databases of chemical and biological reactions
- A Lego-like platform for small molecule synthesis
- Rapid biocatalyst discovery, engineering, and optimization

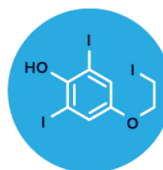
## Infrastructure:

- Cyberinfrastructure for creating and maintaining databases at the National Center for Supercomputing Applications
- Molecule Maker Lab in the Beckman Institute
- Automated synthesizers
- Illinois Biofoundry for Advanced Biomanufacturing (iBioFAB)

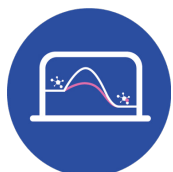
# OUR RESEARCH



**Thrust 1: AI-Enabled Synthesis Planning**



**Thrust 3: AI-Enabled Molecule Manufacturing**



**Thrust 2: AI-Enabled Catalyst Development**



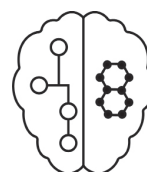
**Thrust 4: AI-Enabled Molecule Discovery**



**Thrust 5: Education and Workforce Development**

## OUR TEAM

The MMLI is a collaboration between the University of Illinois-Urbana Champaign, Rochester Institute of Technology, and Pennsylvania State University. The MMLI is an AI Institute for Molecular Discovery, Synthesis Strategy, and Manufacturing supported by the National Science Foundation.



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moleculemaker.org  
moleculemaker@illinois.edu  
Twitter: @Molecule\_Maker

# INDUSTRIAL PARTNERSHIP PROGRAM

The goal of the MMLI Industrial Partnership Program is to provide the opportunity for the two-way exchange of information between the MMLI and industry researchers.

This program is a way for MMLI researchers to share the tools and databases being developed for more efficient synthesis and discovery of chemical and materials for a wide-range of applications. Industry researchers can provide perspective on which projects will most benefit society.



There is a two-tier membership structure (Partner and Associate), with the annual membership fees going into a seed grant fund to support proof-of-concept projects and expand partnerships.

## **Benefits for all Members:**

- Invitation to the annual MMLI retreat to get a comprehensive overview of the MMLI research
- Recruiting opportunities for graduate students and postdocs
- Opportunity to sponsor directed research projects
- Opportunity to collaborate on other federal grant proposals
- Advertisement of company logo on MMLI website and materials

## **Additional Benefits for Partner Level Members:**

- Non-exclusive, royalty-free non-commercial license of materials developed under the seed grant program
- Quarterly meetings on Zoom to exchange research ideas with MMLI researchers
- A role in selecting which proof-of-concept projects are funded from the seed grant program

## **GET STARTED**

1. Contact MMLI team members for more information:

Director, Huimin Zhao (zhao5@illinois.edu)

Managing Director, Celine Young (chyoung@illinois.edu)

Thrust 1, Jian Peng

Thrust 3, Saurabh Sinha

Thrust 2, Scott Denmark

Thrust 4, Martin Burke

2. All partners will be required to sign a membership agreement and a non-disclosure agreement.