The CATALYSIS SOCIETY of Metropolitan New York
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Wednesday, February 19, 2025 @ NJIT
225 Fenster Hall
323 Dr. Martin Luther King Blvd,
Newark, NJ, 07103

Prof. Tyler Josephson

Chemical, Biochemical, and Environmental Engineering, University of Maryland, Baltimore County

Automated reasoning in chemical science and engineering

Large language models (LLMs) like ChatGPT are powerful text-generation tools. They are increasingly relevant in chemical science and engineering, but are unreliable in solving complex, practical problems faced by scientists and engineers. This is fundamentally about gaps in their *reasoning* capabilities.

In this talk, I will illustrate how engineers solve problems using reasoning skills that go beyond pattern-matching, in which current memorization-based machine learning algorithms excel. I will highlight old and new approaches in AI for reasoning, and highlight opportunities for scientists and engineers to leverage these approaches. Examples from

the AI & Theory-Oriented Molecular Science (ATOMS) Lab at UMBC will be highlighted, including prompting LLMs for chain-of-thought reasoning for solving NMR spectra, writing bug-free software for adsorption calculations using formal theorem provers, and incorporating reasoning tools into methods for discovering equations describing force fields for acid-base interactions.

Speaker Bio

Dr. Tyler R. Josephson is an Assistant Professor in Chemical, Biochemical, and Environmental Engineering at the University of Maryland, Baltimore County. He received his B.S. in Chemical Engineering from the University of Minnesota in 2011 and his Ph.D. in Chemical Engineering from the University of Delaware in 2017, after which he was a postdoctoral associate in the University of Minnesota Chemistry Department until 2020. In 2018, he spent time as a visiting scientist in the Mathematics of AI department at IBM Research. At UMBC, he leads the AI & Theory-Oriented Molecular Science (ATOMS) Lab, developing computational methods for molecular simulation and automated discovery of scientific theories. Techniques used in the ATOMS Lab include quantum chemistry, Monte Carlo, symbolic regression, large language models, and formal theorem proving using Lean. Dr. Josephson received the NSF Graduate Research Fellowship and is the 35th Laird Fellow at the University of Delaware. His research is supported by the National Science Foundation, the Department of Energy, and the Department of Defense, including the NSF CAREER Award for “Automated Reasoning to Advance Chemical Theory” and the Army HBCU/MSI Early Career Award for “Simulation methods for reactive adsorption of emerging water pollutants.”

Schedule		Meeting Fees	
Social Hour	6:30 PM	Non-members	$50
Dinner	7:00 PM	Students	$25 (Student Members = $10)
Presentation	7:30 PM	Retired/Post-Doc/Unemp.	$40 (Members = $30)
		Annual Membership Dues	***$35 (Students = $15)***

There will be no student speaker this meeting

Deadline for reservations is **5:00PM Friday, February 14, 2025**

Please RSVP online using the online form.

To renew your membership, please visit this link.