American Chemical Society

ACS Midland Section

Lunch and Learn Seminar Series

Title: Catalyst Discovery via AI-accelerated Quantum Chemistry and Microkinetic Modeling

Speaker: Dr. Aayush Singh

August 14th,2025
MSU St. Andrews
Midland, MI

Programming Committee:
Judith Espinoza, Allison Abdilla, Raghida Bou Zerdan, Nanguo Liu

ACS Chemistry for Life®

Event flyer

ACS Midland Section Lunch & Learn

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The Future of Chemistry

Catalyst Discovery via AI-accelerated Quantum Chemistry and Microkinetic Modeling

Abstract:
Many grand challenges in the chemical industry, such as CO2 upgrading to jet fuel, methane pyrolysis, plastics upcycling, and low-temperature fertilizer production, are currently limited by the lack of efficient catalysts. Over the past three decades, physics-based simulations leveraging quantum chemistry and microkinetic modeling have enabled high-throughput predictions of catalyst activity and selectivity. However, the high computational cost of quantum chemical methods limits their application in modeling multiscale phenomena, sampling diverse conformational and compositional states, and characterizing materials with intricate electronic properties. At SandboxAQ, we leverage machine learning, generative AI, and multiscale modeling to drastically accelerate physics-based simulations of catalytic reactions. This approach provides new insights into previously inaccessible phenomena such as catalyst stability under reaction conditions. In this presentation, we will compare our AI-accelerated methods to incumbent computational discovery workflows using the example of syngas to multi-carbon products catalyzed by transition metal surfaces—a complex reaction network that depends strongly on catalyst structure and composition.

Aayush Singh
Staff Research Scientist

Speaker Biography
Aayush Singh is a staff research scientist at SandboxAQ, where he leverages AI, quantum chemistry, and microkinetic modeling for catalyst discovery. Aayush received his Ph.D. in Chemical Engineering from Jens Nørskov's group at Stanford University, focusing on computational quantum modeling of catalytic reactions to facilitate the design of a sustainable alternative to the Haber-Bosch process for ammonia production. Aayush then spent five years at Dow Silicones, where he used an array of computational techniques to discover novel catalyst families and simulate complex chemical processes.

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Lunch RSVP

Thursday, August 14th, MSU St. Andrews
11:30 – 12:00pm Lunch & Networking
12:00 – 1:00pm Seminar

Picture 1

August 14th, 2025 MSU St. Andrews, Midland, MI. Introducing our speaker Dr. Aayush Singh, Research Scientist at SandboxAQ by Dr. Allison Abdilla.

Picture 2

August 14th, 2025 MSU St. Andrews, Midland, MI. Our Lunch and Learn speaker after concluding his seminar. Dr. Aayush Singh, Research Scientist at SandboxAQ.

Picture 3

August 14th, 2025 MSU St. Andrews, Midland, MI. Lunch and Learn attendees.