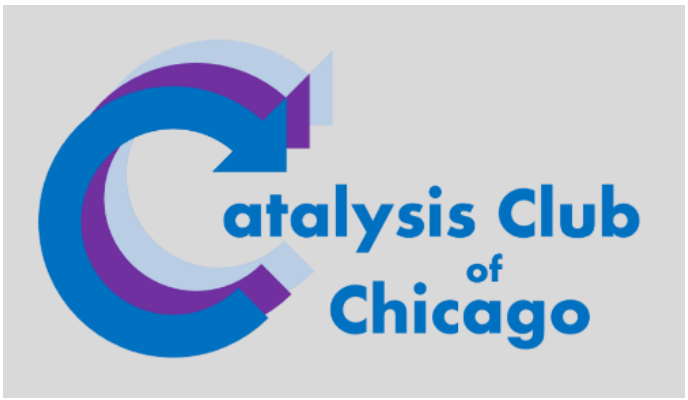

2025 Young Scientist Symposium Program Booklet

January 10, 2025

9:10 AM – 4:15 PM CST

Virtual Meeting, Held via Zoom

2025 Young Scientist Symposium Program

all times listed in CST

Main Zoom Link
https://uwmadison.zoom.us/j/97249113384?pwd=tszpVdnnFaf7J8FkFgb9vCkxexf8H7.1

Meeting ID: 972 4911 3384
Passcode: 166634

Gathertown Poster Session Link
https://app.gather.town/app/5TlmB4pCNPPwNwUc/2025%20CCC%20YSS%20Poster

Morning Session

9:10 **Opening Remarks**

9:15 **Talk A: Selective Hydrogen Combustion over Silica-Supported Sodium Tungstate Catalysts**
Elijah R. Kipp, University of Minnesota – Twin Cities

9:40 **Talk B: Effects of Pd Site Structure and Interconversion on Wacker Oxidation of Ethylene over PdCu/Zeolites**
Deepak Sonawat, University of Wisconsin – Madison

10:05 **Talk C: Quantifying the Kinetics of Framework Dealumination during Hydrothermal Aging of Proton-Form CHA Zeolites**
Tania L. Class-Martinez, Purdue University

10:30 **Break**

10:35 **Talk D: Conductive polymer coating on hydrophobic membrane creates robust gas diffusion layer for electrocatalysis with long-term stability**
Hwiyoon Noh, Purdue University

11:00 **Technical Keynote: Kinetic Barriers to Metal Hydride Complex Formation in Fuel-forming Catalysis**
Prof. Jillian Dempsey, University of North Carolina at Chapel Hill

11:45 **Lunch**

12:15 **Poster Session 1: Even Numbers**
Gathertown

12:55 **Poster Session 2: Odd Numbers**
Gathertown

1:35 **Break**

Afternoon Session

1:40 **Talk E: Selective Hydrogenation of Biomass-derived Furans Over Cu Catalysts: Experiments and Theory**
Evangelos Smith, University of Wisconsin – Madison

2:05 **Talk F: First-Principles Insights into Electrolyte Effects on Electrochemical Reductive Bond Homolysis Selectivity**
Nhu Hue Quach, University of Minnesota – Twin Cities

2:30 **Talk G: Understanding Carrier-dependent (Stereo)-Selectivity in the Dehydrogenation of Liquid Hydrogen Carriers over Metal Catalysts**
Matthew D. Edgar, University of Wisconsin – Madison

2:55 **Break**

3:00 **Talk H: Mechanisms of H_2 Reduction of Cu^{2+} Ions and Implications for Cu Site Distribution in Cu-Exchanged Zeolites**
Jose Rebolledo-Oyarce, University of Notre Dame

3:25 **Career Pathways Panel Discussion: Careers in Academia, National Lab, Industry, Consulting, and Government**
Prof. Jillian Dempsey, UNC
Dr. Felipe Polo-Garzon, Oak Ridge National Laboratory
Dr. Charles Roberts, Toyota
Dr. Sade Ruffin, Booz Allen Hamilton
Dr. David Marchand, BGS for U.S. DOE WPTO

4:10 **Closing Remarks**

Technology Support

Please contact the following person for technical assistance during the meeting:

Morning Zoom Session: (9:10 AM – noon): Sara Ahsan (sahsan3@wisc.edu)

Gathertown Poster Sessions (12:15 – 1:35 PM):

Ciara Tyler (tyler254@umn.edu), Jose Rebolledo Oyarce (jrebolle@nd.edu)

Afternoon Zoom Session (1:40– 4:15 PM): Bereket Bekele (bbekele@purdue.edu)

Keynote: Kinetic Barriers to Metal Hydride Complex Formation in Fuel-forming Catalysis

Abstract. Proton-coupled electron transfer (PCET) processes underpin the catalytic transformations that take energy-poor substrates to energy-rich fuels. Many of these catalytic transformations proceed through metal hydride intermediates. Intriguingly, mechanistic studies undertaken by our lab reveal the PCET reactions that form metal hydride intermediates almost exclusively follow a stepwise electron transfer–proton transfer pathways. Moreover, in several examples, ligands are initially protonated, followed by a tautomerization to yield the stable metal hydride product. The preference for a stepwise reaction over a concerted proton-coupled electron transfer (CPET) route that circumvents the high energy, charged intermediates associated with stepwise pathways, as well as a kinetic preference for protonating the ligand over direct metal protonation, suggests multiple factors dictate the PCET reactions that form metal hydride species. Research in our lab aims to understand the factors underpinning reaction pathways that yield metal hydride complexes.

Prof. Jillian Dempsey

Bowman and Gordon Gray Distinguished Term Professor

Department of Chemistry

University of North Carolina at Chapel Hill

Jillian L. Dempsey is a professor at the University of North Carolina at Chapel Hill where she holds the Bowman and Gordon Gray Distinguished Term Professorship. She is currently the Deputy Director of the Center for Hybrid Approaches in Solar Energy to Liquid Fuels (CHASE), and an associate editor for ACS Electrochemistry.

Jillian received her S.B. from the Massachusetts Institute of Technology in 2005 where she worked in the laboratory of Prof. Daniel G. Nocera. As an NSF Graduate Research Fellow, she carried out research with Prof. Harry B. Gray and Dr. Jay R. Winkler at the California Institute of Technology, receiving her PhD in 2011. From 2011–2012 she was an NSF ACC Postdoctoral Fellow with Daniel R. Gamelin at the University of Washington.

In 2012, Jillian joined the faculty at the University of North Carolina at Chapel Hill. Her research group explores charge transfer processes associated with solar fuel production, including proton-coupled electron transfer reactions and electron transfer across interfaces. Her research bridges molecular and materials chemistry and relies heavily on methods of physical inorganic chemistry, including transient absorption spectroscopy and electrochemistry. She has received numerous awards including the Harry B. Gray Award for Creative Work in Inorganic Chemistry by a Young Investigator (2019), the J. Carlyle Sitterson Award for Teaching First-Year Students (2017), a Sloan Research Fellowship (2016), a Packard Fellowship for Science and Engineering (2015), the Agnes Fay Morgan Research Award (2020), and the University Award for Advancement of Women (2021).

Career Pathways Panel Discussion: Careers in Academia, National Lab, Industry, Consulting, and Government

Dr. Felipe Polo-Garzon

Surface Chemistry and Catalysis Group

Oak Ridge National Laboratory

Felipe Polo-Garzon received his BS in Chemical Engineering from Universidad del Valle (Colombia) and received his PhD in Chemical Engineering from Clemson University (United States). In 2016, he joined Oak Ridge National Laboratory (ORNL) as a Postdoctoral researcher in the Surface Chemistry and Catalysis Group in the Chemical Sciences Division. Later, he became a R&D Staff within the same group. His research interests deal with the development of reactivity descriptors for heterogeneous catalysis, as well as the elucidation of governing reaction mechanisms through *in-situ* and *operando* characterization techniques, kinetic analysis and computational tools. His expertise includes acid-base catalysis, polymer upcycling, as well as natural gas upgrading (selective hydrogenation, methane combustion, coupling and reforming). He is Thrust Lead of the DOE Catalysis Program at ORNL "Fundamentals of Catalysis and Chemical Transformations" and co-PI of the DOE Energy Earthshot Research Center "Non-Equilibrium Energy Transfer for Efficient Reactions (NEETER)". He is recipient of UT-Battelle Award "Team Award for Outstanding Research Output in Science & Technology" (2023), and the Luminary Award by Great Minds in STEM (GMiS) (2024).

Dr. Charles A. Roberts

Senior Research Manager - Catalytic Materials

Toyota Research Institute of North America

Dr. Charles "Chip" A. Roberts is the Senior Research Manager of the Catalytic Materials Lab in the Materials Research Department of the Toyota Research Institute of North America (TRINA) in Ann Arbor, MI. He graduated from the University of Notre Dame with a B.S. in Chemical Engineering and received a Ph.D. in Chemical Engineering from Lehigh University, where he utilized *in situ* and *operando* optical spectroscopy to study photocatalytic water splitting. He joined TRINA within Toyota Motor North America R&D in 2012, where his research has focused on automotive exhaust gas purification, with a specific focus on the identification of structure-function-reactivity relationships for deNO_x reactions over metal oxide catalysts utilizing

spectroscopic characterization. His work was among the first in TRINA to include the application of machine learning methodologies to support experimental optimization and discovery of new material compositions; namely, metal oxide catalysts for direct decomposition of NO_x to N_2 and O_2. He manages a diverse group of researchers who are all striving to enable electrification and carbon neutrality in the mobility industry by performing materials research for fuel cell, emission catalyst, and carbon capture & utilization. While at Toyota, he has fostered connections between industry and academia, not only through direct research collaboration with universities & national laboratories, but also by supporting the first TRINA "Visiting Scholar" position to facilitate an on-site industrial research experience for a professor. He remains active in the catalysis community with the Michigan Catalysis Society, the North American Catalysis Society as member of the technical program committee for NAM28, and AIChE as Director of the Catalysis & Reaction Engineering Division.

Dr. Sade Ruffin

Senior Lead Engineer

Booz Allen Hamilton

Dr. Sade Ruffin is a Senior Lead Engineer at Booz Allen Hamilton, where she works with clients to identify cutting-edge energy R&D opportunities, define state-of-the-art technologies, and makes strategic recommendations for transformational programs driving innovation. Through this work she has contributed to programs with a strong need for catalyst expertise. Some examples include programs focused on accelerating the development of heterogeneous catalysts for net-zero emissions and resource recovery from wastewater. Dr. Ruffin holds a PhD in Chemical Engineering from NYU where she focused on surface chemistry. With her background she has also lead work on advanced catalyst systems. Prior to Booz Allen Hamilton, she worked at Cummins Emissions Solutions, where she performed root cause analysis and characterization studies related to aftertreatment systems and technologies. Throughout her career, Sade has leveraged her technical expertise and strategic insight to help organizations advance transformative projects aligned with global sustainability goals.

Dr. David Marchand

Commercialization Analyst

Boston Government Services, Contractor to U.S. DOE Water Power Technologies Office

David Marchand is a Commercialization Analyst for the U.S. Department of Energy's Water Power Technologies Office (WPTO). He leads WPTO's SBIR (Small Business Innovative

Research) program and supports the office's portfolio of technology commercialization projects. Prior to joining WPTO in November 2023, David founded a start-up to develop plant-based, biodegradable coatings as a sustainable replacement for plastics in food packaging. He also has five years of experience in the engineering, sales, and marketing of materials characterization instrumentation. David holds a B.S. in Chemical Engineering & Materials Science from Lehigh University and a Ph.D. in Chemical Engineering from The Pennsylvania State University. He is based in Washington, D.C.

Young Scientist Symposium Posters

Note: Poster presenters should be at their poster for one of the two sessions; even numbers will present at 12:15 PM CST, odd numbers will present at 12:55 pm CST

Poster Session Link:

Poster #	Title & Authors
1	**Studies of CO_2 hydrogenation over Cu on alumina supported transition metal nitrides and carbides** Dr. Siobhan W. Brown, Northwestern University
2	**Consequences of Confinement and Acid Strength on Arene Methylation Kinetics and Product Selectivities over Acidic Zeolites** Andrew T. Norfleet, Purdue University
3	**Investigating the Evolution and Consequences of Heterogeneous Cu Sites on Stoichiometric Partial Methane Oxidation in Cu-CHA Zeolites** Lauren Kilburn, Purdue University
4	**Understanding Reactant-Induced Sintering in the Hydrogenation of Liquid Hydrogen Carriers over Metal Catalysts** Sara Ahsan, UW-Madison
5	**Investigating the Sulfur Poisoning Characteristics of High-Entropy Alloys Using a Multi-Property Graph Neural Network** Dr. Gaurav S. Deshmukh, Northwestern University
6	**Synthesis and Characterization of Structurally Stable Molybdenum-Zeolite Catalysts for Methane Dehydroaromatization** Ángel N. Santiago Colón, Purdue University
7	**Unraveling Temperature-Dependent Free-Energy Landscapes and Surface Dynamics in Methane Activation on Ni(511) via Machine Learning and Enhanced Sampling** Yezhi Jin, The University of Chicago
8	**Room temperature C—H bond activation of propane on Pt electrocatalyst in aqueous acidic electrolyte** Ashutosh Bhadouria, Purdue University

9	**Synthesis of MFI Zeolites with Small Crystallite Sizes to Generate Stable Product Selectivity from Alkene Oligomerization** Dr. Sanghyun Ahn, Purdue University
10	**Synthetic Methods to Control the Siting of Trivalent Heteroatoms in MFI Zeolite Channels for Selective Toluene Methylation to p-Xylene** Bereket T. Bekele, Purdue University
11	**Identifying Methanol Adsorbate Geometries on (101)-Faceted Anatase Titania Nanocrystals** Dr. Benjamin M. Moskowitz, PNNL
12	**Reduction pathway selectivity for nitrous oxide selective catalytic reduction over Fe-zeolites** Elizabeth A. Brungardt, UW-Madison
13	**The Impact of Acid-site Pairing on Adsorption and Reactivity in CHA** Nikki Kragt, University of Florida
14	**Proximity Control of Active Sites to Facilitate Tandem Catalysis in Propane Oxidative Dehydrogenation** Dr. Geunho Han, Northwestern University
15	**Microenvironment Engineering to Fine-tune Selectivity of the Electrochemical CO_2 Reduction on a Copper-Gold Catalyst** Seyed Parsa Amouzesh, Illinois Institute of Technology
16	**Integrating Earth-Abundant Iron in Metal-Ligand Single Atom Catalysts for Propane Dehydrogenation** Dr. Wondemagegn H. Wanna, Indiana University
17	**Quantifying Rates and Active Sites in Carbon Surfaces that Catalyze Non-oxidative Coupling of Methane** Justin E. Rosa-Rojas, Purdue University
18	**Measuring Dispersion of Zr-SiO_2 with *in situ* Titration** Emily K. Chase, Northwestern University
19	**Assessing the Influence of Acid Site Location in MFI Zeolites on Propene Oligomerization Rates and Selectivity** Diamarys Salome Rivera, Purdue University
20	**Hydroxide Ion Conduction through Viologen-based Covalent Organic Frameworks (vCOFs): an Approach towards the Advancement** Pampa Jhariat, Vellore Institute of Technology
21	**Interrogating the Kinetic and Mechanistic Origins of N_2O Formation during NH_3 Selective Catalytic Reduction of NO_X on Cu-CHA Zeolites** Bryan L. Cruz Delgado, Purdue University
22	**Deactivation, Site Requirements, and Product Inhibition over Au/TS-1 Bifunctional Propene Epoxidation Cascades** Ryoh-Suke Sekiya, Purdue University
23	**Microkinetic modelling of ethylene oligomerization on H-BEA zeolites** Dr. Sai Praneet Batchu, Northwestern University

Acknowledgements

The Catalysis Club of Chicago would like to thank the following people for their generous contributions to the success of the 2025 Young Scientist Symposium, including:

CCC Institutional Representative Committee:

- Bereket Bekele (Purdue)
- Seryeong Lee (Northwestern)
- Minjung Kim (Northwestern)
- Dawson Grimes (Northwestern)
- Sara Ahsan (UW-Madison)
- Carly Byron (Argonne National Lab)
- Ciara Tyler (U. Minnesota)
- Jose Rebolledo-Oyarce (U. Notre Dame)

Abstract Reviewers:

- Chris Keturakis, Siddarth Krishna, Rajamani Gounder, Patrick Littlewood

Talk and Poster Judges:

- Brian Tackett, Matthew Kline, Phuong Do, Siddarth Krishna, Lijun Xu, Christopher Nicholas, Felipe Polo-Garzon, Robert Carr, Eric Sacia, Evan Wegener, Eric Moschetta, Brandon Vance, Zhanyong Li, Patrick Littlewood, Marcel Schreier, and William Schneider