UC Chemical SYMPOSIUM

Sept. 7th-9th 2025

www.ucchemsym.org @UCChemSym

Table of Contents

Welcome

Welcome to the 2025 University of California Chemical Symposium! The 2025 UCCS is held on September 7-9, 2025 at the UCLA Lake Arrowhead Conference Center and will be attended by almost 80 University of California undergraduates, graduate students, and postdoctoral scholars. As the UC system is home to some of the most cutting edge research in the chemical sciences, we encourage you all to exchange research ideas with your peers from other campuses, explore future career options with our guest senior scientists, and engage in our professional development workshops. It is our hope that lasting research and personal relationships will be formed through this conference.

In this document you will find all of the information you will need for the conference. You may also refer to our website for more information, and we encourage you to follow us on X @UCChemSym and share your photos during the meeting!

The UCLA Lake Arrowhead Conference Center and Transportation

The UCLA Lake Arrowhead Conference Center is located in Lake Arrowhead, California. This venue has a secluded mountain-retreat feel with all meals and cottage-style Condolets provided. Outside of the conference there are many opportunities for recreation such as local ski resorts and hiking trails.

Directions to the UCLA Lake Arrowhead Conference Center can be found on their website. If you are flying into Ontario Airport please note that there is still a considerable drive to the conference venue (approximately 1 hr).

For most routes: Take Freeway 210 east (Mountain Resorts). Exit at Waterman Avenue and turn left (North) at signal. Continue forward. Waterman Avenue turns into Highway 18. Stay on Highway 18 for 20 miles into the mountains to the Lake Arrowhead turnoff. This is a left turn

onto Highway 173. Stay on Highway 173 for approximately 2 miles until you come to a stop sign. Turn right at the stop sign. This is a continuation of Highway 173. You will be on Highway 173 for approximately 5 miles around the lake. When you see our sign (UCLA Conference Center) take the very next left onto Willow Creek Rd. Come to the end of the road, curve to the right, and then take the next right into the Conference Center.

Address: UCLA Lake Arrowhead Conference Center
850 Willow Creek Rd, Lake Arrowhead, CA 92352

UCLA LAKE ARROWHEAD CONFERENCE CENTER PROPERTY MAP

IACC CERTIFIED VENUE

UCLA LAKE ARROWHEAD CONFERENCE CENTER

P.O. Box 160 • 850 Willow Creek Road
Lake Arrowhead, CA 92352
(909) 337-2478
LakeArrowhead.ucla.edu

6/16

Check-in

Please check-in to your rooms between 4:00 PM and 5:00 PM on Sunday, September 7th. There will be a booth set-up through the main entrance at the Main Lodge. From there you will receive your conference materials and room assignment. Our opening address begins promptly at 5:00 PM, followed by the opening keynote at 5:30 PM, dinner at 6:30 PM, and lightning talks at 8:00 PM.

Check-out

The conference will conclude on Tuesday, September 9th, at 12:00 PM. Please check-out by returning your key to the front desk **before 11:00 AM**. Lunch will be provided from 12:00-1:00 PM prior to our departure at 1:00 PM.

Presentation Guidelines

Posters

Posters should be no larger than 3' × 4' (36” × 48”) which is the same size as ACS posters. You will be assigned a poster number, and given the supplies and location to mount your poster. Please mount your posters between 8:00 and 8:30 PM on Monday, September 8th. The poster session will begin at 8:30 PM.

Platform Talks

Talks should be 12-15 minutes long, with 3-5 minutes of this time allotted for questions. Please bring your own computer with a HDMI adapter. Oral presentations will take place during a morning session (9:00 AM - 12:00 PM) and an afternoon session (4:30 - 6:30 PM) on Monday, September 8th.

Lightning talks

Lightning talks should be about 3 minutes long (typically 2 or 3 slides), with 2 minutes for questions. These are sent to the organizing committee in advance of the conference so they can be collated and pre-loaded for smooth transition between talks. The lightning talk session will begin promptly at 8:00 PM on Sunday, September 7th.

Awards

Best Platform Talk	*Chemical Communications*
Best Poster	*Materials Horizons*
Best Flash Talk	*RSC Advances*
Environmental & Analytical Division Award	*Environmental Science*
Biochemistry & Chem Bio Division Award	*RSC Pharmaceutics*
Inorganic Division Award	*Dalton Transactions*
Organic Division Award	*Organic & Biomolecular Chemistry*
Physical Division Award	*RSC Mechanochemistry*
Materials Division Award	*Materials Advances*

Conference Schedule

Sunday, September 7

4:00 - 5:00 PM	Arrival, Check-In, and Registration	Main Lobby
5:00 - 5:30 PM	UCCS 2025 Opening Remarks	Pineview
5:30 - 6:30 PM	**Ursa Keynote: Elizabeth Neumann**	Pineview
6:30 - 8:00 PM	Welcome Dinner	Dining Room
8:00 - 9:00 PM	Lightning Talk Session	Pineview
9:00 - 11:00 PM	Networking Social & Drinks	Lakeview

Monday, September 8

8:00 - 9:00 AM	Breakfast	Dining Room
9:00 - 12:00 PM	Platform Talks	
	Pineview Session A	Pineview
	Lakeview Session A	Lakeview
	Library Session A	Library
12:00 - 1:00 PM	Lunch	Dining Room
1:00 - 2:00 PM	Afternoon Break	
2:00 - 3:15 PM	**Workshop A** How to Publish With Impact	Lakeview
	Workshop B What it means to Connect	Pineview
3:15 - 4:30 PM	Career Panel	Pineview
4:30 - 6:30 PM	Platform Talks	
	Pineview Session B	Pineview
	Lakeview Session B	Lakeview
	Library Session B	Library
6:30 - 8:00 PM	Dinner	Dining Room
8:30 PM - 11:00 PM	Poster Session & Drinks	Pineview Lakeview

Tuesday, September 9

8:00 - 9:00 AM	Breakfast	Dining Room
9:30 - 10:30 AM	Break - Check Out	
10:30 - 11:30 AM	**Lux Keynote: Akif Tezcan**	Pineview
11:30 - 12:00 PM	Closing Address and Awards Session *Sponsored by RSC*	Pineview
12:00 - 1:00 PM	Lunch	Dining Room

Professional Development Activities

Career Panel

Do you struggle to answer the dreaded question about your plans after graduation? Come to the career panel to get some ideas of what career options you have. The career panel will take place on Monday, September 8th from 3:15 - 4:30 PM in the Pineview Room. Please come prepared with your career questions and note that there will be time to interact with these individuals throughout the conference.

Meet the Panelists

Prof. Trevor Bolduc - UC Riverside

Trevor is an assistant professor of teaching at UC Riverside, specializing in chemical education in organic chemistry. Before joining UCR, he completed his PhD with Prof. Glenn Sammis at the University of British Columbia, Vancouver where he investigated the synthetic applications of sulfuryl fluoride and thionyl fluoride as reagents for fluorination chemistry. Trevor is interested in alternative grading and assessment design in his courses, as well as the use of app-based learning technologies in undergraduate organic chemistry. He is in charge of the sophomore organic chemistry labs at UCR, where he is in the process of redesigning the curriculum and streamlining content delivery for students and the teaching team.

Prof. Elizabeth Neumann - UC Davis

The Neumann lab joined the Chemistry Department at UC Davis in the summer of 2022 and focuses on understanding the molecular and cellular architecture behind neurological diseases. The research is highly interdisciplinary and involves developing analytical tools and multimodal imaging methods for understanding complex biological phenomena. In sum, we use matrix-assisted laser desorption/ionization mass spectrometry imaging (MALDI MSI) to measure hundreds to thousands of molecular features within a biological sample without disturbing their spatial content. We can then couple this chemically informative information to other powerful technologies, such as highly multiplexed immunofluorescence , spectroscopy, or transcriptomics, to get a more complete picture of complex biological systems. We are always looking for enthusiastic and passionate students to join as well as collaborators in any field for collaboration, as these approaches are applicable to most biological systems. Elizabeth Neumann was an NSF doctoral fellow at the University of Illinois at Urbana Champaign and an NIH postdoctoral fellow at Vanderbilt University.

Prof. Rex Handford - UC Irvine

Originally from Burnaby, British Columbia, Canada, Rex studied chemistry as an undergraduate at the University of British Columbia. Under the tutelage of Prof. Peter Legzdins, he fell in love with inorganic and organometallic synthesis. Rex went on to pursue graduate studies with Prof. T. Don Tilley at UC Berkeley, where he developed new methods to access molecular complexes possessing "bare" silicon atoms, which resemble catalytically-active metal-silicon phases. As a postdoctoral fellow, Rex examined the behavior and reactivity of mixed-metal clusters with Prof. Theodore Betley at Harvard University, characterizing the effect of metal-metal cooperativity in polynuclear active sites. In Summer of 2025, Rex began his independent career as an assistant professor within the Department of Chemistry at UC Irvine. This lab is focused on designing expanded inorganic molecules that capture the reactive elements of metal-metal and metal-element bonds found in heterogeneous catalysts and bioinorganic active sites.

Dr. Joseph Palasz - Lawrence Berkeley National Laboratory

Dr. Joseph Palasz is a postdoctoral researcher at Lawrence Berkeley National Laboratory (LBNL) in Berkeley, California. He completed his undergraduate degree at Northwestern University in the Integrated Science Program (ISP) with a thesis studying solution processable solar devices with Professor Samuel I. Stupp. He received his PhD from University of California San Diego in 2024 working with Professor Clifford P. Kubiak studying electron transfer dynamics in organometallic complexes. He is currently working on developing scalable chemical pretreatment steps for lignocellulosic biomass to enable the conversion of agricultural waste streams into fermentable sugars and valuable bio-based starting materials for chemicals and materials production. His research interests include (1) green chemical transformations (2) materials synthesis starting from biomass derived substrates (3) imaging and spectroscopy of biological and synthetic material systems and (4) electrochemical and photochemical reactions. His research profile is available at: https://orcid.org/0000-0002-9825-6981

Prof. Akif Tezcan - UC San Diego

Akif Tezcan is a Professor in the Department of Chemistry and Biochemistry and a member of the Materials Science and Engineering (MSE) Program and the Institute of Materials Discovery and Design at UCSD. He was educated at the German High School in Istanbul, Macalester College in St. Paul, MN (BA in Chemistry and Biology) and Caltech in Pasadena, CA, USA (PhD in Bioinorganic Chemistry with Harry Gray), followed by postdoctoral research at Caltech as a Helen Hay Whitney fellow (with Doug Rees). His research program at UCSD, started in 2005, focuses on developing new chemical tools and strategies to study biological nitrogen fixation, to design functional proteins and enzymes, and to create new protein-based materials.

Workshops

Workshop A: How to Publish With Impact

Lakeview (Zoom: https://uci.zoom.us/j/96853531834), 2:00 - 3:15 PM

This workshop on impactful dissemination of research will describe the scientific publishing process, some advice for writing effective papers, and tips and tricks on promoting the work once it is published. Some ethical considerations, particularly around the use of AI in science writing, will also be discussed.

Presented by James White, Royal Society of Chemistry

> *James White is a Content Development Editor with the Royal Society of Chemistry based in the Washington, DC office. Researching carbon dioxide electrochemistry, he earned his Ph.D. in Chemistry and Materials from Princeton University, and he subsequently studied solid-state hydrogen storage at Sandia National Laboratories in Livermore, California as part of the Hydrogen Materials-Advanced Research Consortium (HyMARC). He has worked in scientific editing and publishing for the past five years.*

Workshop B: 'What it means to Connect'

Pineview, 2:00 - 3:15 PM

An interactive networking workshop to discuss building, maintaining, and leveraging your professional network in graduate school while creating friendship bracelets.

Keynote Speakers

Ursa Lecture

Prof. Elizabeth Neumann

Assistant Professor, Department of Chemistry, UC Davis

Organ systems are composed of unique cell types that actively coordinate to enable higher order functions. Even slight deviances in the molecular or cellular states of these systems can result in debilitating disorders whose severity, treatment course, and overall treatment outcome vary widely from patient to patient. This level of complexity likely contributes to promising therapeutics failing within clinical trials and, thus, require further exploration. Thus, the Neumann lab focuses on developing and applying multimodal imaging and profiling techniques to study complex human diseases, such as renal cell carcinoma, Alzheimer's Disease, and spina bifida. Beyond disease, we also develop methods for spatially assessing exogenous agents, including pharmaceuticals, toxins, and plastics, within organ and whole animal models.

Selected Awards and Honors

- 2019 ASMS Asilomar Travel Award
- Vanderbilt Dr. Laura Busenlehner Award for outstanding postdoctoral trainee for discovery science
- NIH Toxicology Institutional National Research Service Award (T32)
- NIH NIDDK Postdoctoral Individual National Research Service Award (F32)
- 2019 ACS Partners for Progress and Prosperity Award
- 2019 UIUC Graduate Student Leadership Award
- National Science Foundation Graduate Research Fellowship
- UIUC Springborn Endowment Fellowship
- UIUC Illinois Distinguished Fellowship

Lux Lecture

Prof. Akif Tezcan

Professor, Chemistry and Biochemistry, UC San Diego

Proteins represent the most versatile building blocks available to living organisms or the laboratory scientist for constructing functional materials and molecular devices. Underlying this versatility is an immense structural and chemical heterogeneity that renders the programmable self-assembly of proteins an extremely challenging design task. To circumvent the challenge of designing extensive non-covalent interfaces for controlling protein self-assembly, our group has endeavored to use chemical bonding strategies based on fundamental principles of inorganic chemistry and molecular symmetry. These strategies (combined with some supramolecular and polymer chemistry) have resulted in discrete or infinite, 0-, 1-, 2- and 3D protein architectures that display high structural order over large length scales, yet are dynamic, adaptive and possess new emergent chemical/physical properties. In this talk, I will present some of these functional “bioinorganic materials” constructed in our laboratory.

Selected Awards and Honors

- 2026 ACS Alfred Bader Award in Bioinorganic or Bioorganic Chemistry
- 2024 UC Davis Louis R. Gomberg Lecturership
- 2023 University of New Mexico Riley Schaeffer Endowed Lectureship in Chemistry
- 2021 Guggenheim Fellow
- 2016 Caltech Ernest H. Swift Lectureship
- 2015 Kavli Frontiers Fellow
- 2014 SBIC Early Career Award
- 2014 Caltech Moore Distinguished Scholar
- 2012 Frasch Foundation Award
- 2011 Saltman Lecture Award, GRC Metals in Biology
- 2010 Sloan Research Fellowship
- 2008 Beckman Young Investigator Award
- 2007 NSF CAREER Award

2025 UCCS Organizing Committee

Prof. Alexander Spokoyny	*UC Los Angeles*	Faculty Advisor
Prof. Rebeca Arevalo	*UC Merced*	Faculty Advisor
Vicki Rubio	*UC Los Angeles*	Co-chair
Jae Elise Payong	*UC Irvine*	Co-chair
Ashley Pimentel	*UC Riverside*	Website and Social Media
Mei Matsumoto	*UC Los Angeles*	Finances
Amanda Caceres	*UC Davis*	Programming
Riley Blue	*UC Santa Cruz*	Venue Liaison
Elisa Olivas	*UC Irvine*	Flex
Yueying “Qiao-Qiao” Wang	*UC Los Angeles*	Flex

Future 2026 UC Chemical Symposium Committee Selection

If you would like to help organize the next UCCS, please fill out our post-conference evaluation and indicate that you would be interested in participating! Alternatively, you may email the UC Chemical Symposiun (ucchemsym@gmail.com) or Prof. Alexander Spokoyny (spokoyny@chem.ucla.edu).

2025 Sponsors

We are very grateful to all of our sponsors for their support and making this conference possible.

University of California Sponsors

UC MERCED

UC RIVERSIDE

UCI

UCLA

UC SANTA CRUZ

UC SANTA BARBARA

Berkeley
UNIVERSITY OF CALIFORNIA

UC San Diego

Outside Sponsors

ROYAL SOCIETY OF CHEMISTRY

Presentation Schedule

Lightning Talks

Pineview
Sunday, September 7th, 8:00 PM
Moderator: Vicki Rubio

Time	Presenter	Title
8:00 PM	**Hernán Gómez**	Covalent inhibitors of lecithin:retinol acyltransferase (LRAT), an essential enzyme in the visual cycle
8:07 PM	**Piyusha Lotlikar**	Exploration of the photochemistry of Ru(II) complexes with bidentate S donors
8:14 PM	**Shruti Jain**	Photovoltage of BiVO4 Photoelectrode Junctions from Applied Bias Vibrating Kelvin Probe Measurements
8:21 PM	**Yin Pok Wong**	Catalyst repurposing with network science across dissimilar reaction domains
8:28 PM	**Daniel Kendall**	Phenylacetaldehyde photolysis: Modeling toluene's understudied atmospheric oxidation pathway
8:35 PM	**Esveidy Oceguera**	Efficiency of SPhos Oxidative Addition Complex (OAC-2) in Suzuki-Miyaura Cross Couplings

Platform Talks

Session 1: Monday, September 8th, 9:00 AM - 12:00 PM

Pineview A
Organic Chemistry
Moderator: Elise Payong

Time	Presenter	Title
9:00 AM	**Diksha Sharma**	Hydrodefluorination of Polyfluorinated Arenes Catalyzed by Iron-Complex
9:20 AM	**Harsh Chavda**	Indole Photocatalysts and Secondary Amine Ligands Enable Nickel Photoredox C(sp2)−Heteroatom Couplings
9:40 AM	**Partho Paul**	Redox Potential Modulation of Quinones via Intramolecular Hydrogen Bonding for CO_2 Capture applications
10:00 AM	**COFFEE BREAK**	
10:20 AM	**Silvia Rivera**	Diversity-oriented photobiocatalytic synthesis via stereoselective three-component radical coupling
10:40 AM	**Nathan Coddington**	Nickel-Catalyzed C-CN Coupling of Benzonitriles and Cyclopropyl Ketones
11:00 AM	**COFFEE BREAK**	
11:20 AM	**Rajib Mandal**	New-to-Nature Hydrogenases for the Asymmetric Reduction of Unactivated Olefins
11:40 AM	**Pauline Bianchi**	How subtle interactions drive selectivity in intramolecular cyclizations: A computational insight

Lakeview A
Biochemistry and Chemical Biology
Moderator: Ashley Pimentel

Time	Presenter	Title
9:00 AM	**Zoe Heidersbach**	Co-Oligomerization of Alpha- and Beta-Synuclein with Epigallocatechin Gallate
9:20 AM	**An Pham**	Unraveling Excited-State Behavior in Tetrazole Scaffolds for the Functional Design of Selective Peroxynitrite Probes
9:40 AM	**Devon Stuart**	“Turn-On” Sialic Acids for Noncovalent Cell Surface Labeling
10:00 AM	**Samantha Ono**	Development of Surface-Enhanced Raman Probes for the Detection of Heterogeneous Disease Biomarkers
10:20 AM	**COFFEE BREAK**	
10:40 AM	**Julia Balsamo**	Mechanistic Insight into Intestinal α-Synuclein Aggregation in Parkinson’s Disease
11:00 AM	**Zulfiqar Mohamedshah**	Highly Efficient Expression of DNA-peptide Conjugates in Growth-arrested Cells
11:20 AM	**Preeta Pratakshya**	Backbone-modified proteins as functional biomaterials
11:40 AM	**Lilian Zeinalvand**	Understanding the Structure and Dynamics of Peptide-Based Coacervates with In-Situ Liquid and Cryo-TEM

Library A
Inorganic Materials
Moderator: Elisa Olivas

Time	Presenter	Title
9:00 AM	**Elisa Olivas**	The Role of Enzyme Spatial Distribution in Enzyme Metal-Organic Frameworks using Cryogenic Electron Energy Loss Spectroscopy (cryoEELS), & Energy-Filtered TEM (EF-TEM)
9:20 AM	**Linus Murphy**	Simulation Development for HgTe Quantum Dot Growth
9:40 AM	**Bradley Kroes**	Rapid, scalable, and novel methodology for producing graphene-coated silicon microparticles
10:00 AM	**COFFEE BREAK**	
10:20 AM	**Hashim Al Khunaizi**	Approaching the Limit: Boron Clusters as Platforms for Superhydrophobic Coatings
10:40 AM	**Daniel Valenzuela**	Probing the Hot Carrier Activity and Redox Surface Properties of Gold Nanoparticles
11:00 AM	**COFFEE BREAK**	
11:20 AM	**Gilad Gani**	Surface Modifications Using Reductive Desorption of Carborane Monolayers
11:40 AM	**Srijita Pal**	Probing the surface chemistry of porous materials with reactive organic dyes

Session 2: Monday, September 8th, 4:30 PM - 6:30 PM

Pineview B
Inorganic Chemistry
Moderator: Elise Payong

Time	Presenter	Title
4:30 PM	**Jake Stofan**	Synthesis and Reactivity of Mo Complexes Bearing the Redox-Active dppBIAN Ligand Across Several Oxidation States.
4:50 PM	**Tyler Kerr**	A Highly Crystalline Dodecaborate Radical?
5:10 PM	**COFFEE BREAK**	
5:30 PM	**Madison Esposito**	Low-valent metal-organic materials with group 9 metals and phosphine ligands
5:50 PM	**Ye Wen**	Understanding Hardness Mechanisms in Metal Dodecaborides Using Machine Learning Modeling and Simulations
6:10 PM	**COFFEE BREAK**	

Lakeview B
Environmental Chemistry
Moderator: Ashley Pimentel

Time	Presenter	Title
4:30 PM	**Aaron Palmisano**	Exploring Aerosol Chemistry on Prebiotic Earth using Single Particle Levitation
4:50 PM	**Md Shaihan Bin Iqbal**	Photochemically enhanced burn rate of solid propellant
5:10 PM	**Kam Tung Chan**	Nitrate Photolysis in Solution from First Principles Molecular Dynamics and Machine Learning
5:30 PM	**Pedro De Allende**	Exploring the Optical Properties of Brown Carbon Aerosol Using Single Particle Levitation
5:50 PM	**William Ragen**	Optical & chemical transformations from day- and night-aged nitrate-oxidized pyrrole brown carbon aerosols
6:10 PM	**Casey Tsai**	Modeling XFEL Experimental Design For Protein Reaction Studies Using Droplets

Library B
Organic Materials
Moderator: Elisa Olivas

Time	Presenter	Title
4:30 PM	**Marvin Santiago**	Degradable poly(N-vinylpyrrolidone) synthesis in water: advancing green polymer chemistry
4:50 PM	**Riya Singh**	Polymerization-Induced Condensation (PICON)
5:10 PM	**Tommy Frisch**	Renewable and Biodegradable Polyurethanes as Alternatives for Commercial Plastics
5:30 PM	**Takashi Kaneko**	Radical-Free Digital Light Processing of Hydrogels via Photo-Caged Cyclopentadiene Diels–Alder Click Chemistry
5:50 PM	**Joseph Palasz**	Boiling Trees: Using Basic Organic Chemistry to Unlock Lignocellulosic Biomass
6:10 PM	**Adrian Huang**	Cooperative Capture of CO2 from Air with Molecular Polyamine Network Solids

Poster Presentations

Pineview and Lakeview

Monday, September 8th, 8:30 PM

Poster #	Name	Title
1	**Bradley Kroes**	Rapid, scalable, and novel methodology for producing graphene-coated silicon microparticles
2	**Daniel Kendall**	Phenylacetaldehyde photolysis: Modeling toluene's understudied atmospheric oxidation pathway
3	**Erika Chambers**	Enantioselective Alkylation of Cycloalkyl Pyridines with Chiral Lithium Amides as Traceless Auxiliaries
4	**Esveidy Oceguera**	Efficiency of SPhos Oxidative Addition Complex (OAC-2) in Suzuki-Miyaura Cross Couplings
5	**Gilad Gani**	Surface Modifications Using Reductive Desorption of Carborane Monolayers
6	**Hernan Gomez**	Covalent inhibitors of lecithin:retinol acyltransferase (LRAT), an essential enzyme in the visual cycle
7	**John Saunders**	Sustainable Amination and Amidations in Continuous Plug Flow
8	**Juancarlos Rojas**	Sustainable Catalysis: Earth abundant metals for a greener future
9	**Julia Balsamo**	Mechanistic Insight into Intestinal α-Synuclein Aggregation in Parkinson’s Disease
10	**Kam Tung Chan**	Nitrate Photolysis in Solution from First Principles Molecular Dynamics and Machine Learning
11	**Katia Hatem**	Direct Measurements of Criegee Intermediates Using Cavity Ringdown Spectroscopy for the Ozonolysis of a Series of C6 Alkenes
12	**Adrian Jiajin Huang**	Cooperative Capture of CO2 from Air with Molecular Polyamine Network Solids
13	**Luke Jackson**	Carborane Ligated Iridium Hydride Cluster Enables Recyclable Solution Phase Crabtree Type Hydrogenation
14	**Marvin Santiago**	Degradable poly(N-vinylpyrrolidone) synthesis in water: advancing green polymer chemistry

15	**Min Kyu Lee**	Development of Biodegradable Thermoplastic Elastomers for Single-Use Medical Devices: A Sustainable Alternative to Conventional Polymer
16	**Nehal Idris**	Understanding the Encapsulation Behavior of Nile Red within Nonionic Block Copolymer Coacervates and Self-assembled Particles
17	**Parian Poorjafari Jafroodi**	Evaluating Hole Scavenging Efficiency in Metal Nanoparticle Photocatalysis
18	**Piyusha Lotlikar**	Exploration of the photochemistry of Ru(II) complexes with bidentate S donors
19	**Rajib Mandal**	New-to-Nature Hydrogenases for the Asymmetric Reduction of Unactivated Olefins
20	**Riya Singh**	Polymerization-Induced Condensation (PICON)
21	**Sara Murphy**	Effects of Functional Groups on Product Distributions in RO2 + RO2 Reactions
22	**Shruti Jain**	Photovoltage of BiVO4 Photoelectrode Junctions from Applied Bias Vibrating Kelvin Probe Measurements
23	**Takashi Kaneko**	Radical-Free Digital Light Processing of Hydrogels via Photo-Caged Cyclopentadiene Diels–Alder Click Chemistry
24	**Tianren Zhang**	Expanding the Scope of NASICONs to Ammonium Transition Metal Diphosphates
25	**Timothy Chau**	Computational Study of Water's Effect on Isoprene-Derived Peroxy Radical Hydrogen Shift Reactions
26	**Victor de Sousa**	Influence of Ligand Cross-Link Length on Secondary Building Unit Formation in OligoMOFs
27	**Vivek Vasudev**	A new class of photochromes for ultrastable switching and photomechanical motion
28	**Vivian Yuen**	Synthesis and Characterization of Trimetallic Complexes containing Triptycene-based Redox-Active Ligands
29	**Yin Pok Wong**	Catalyst repurposing with network science across dissimilar reaction domains
30	**Zoe Heidersbach**	Co-Oligomerization of Alpha- and Beta-Synuclein with Epigallocatechin Gallate

31	**Preeta Pratakshya**	Backbone-modified proteins as functional biomaterials

Abstracts

Listed in alphabetical order of first name

Aaron Palmisano	**Exploring Aerosol Chemistry on Prebiotic Earth using Single Particle Levitation**	Aerosol particles play a crucial role in the atmosphere, impacting climate, air quality, human health, and planetary processes. Aerosol behavior is driven by their composition and environmental factors, such as relative humidity (RH) and temperature, which influence particle size, refractive index, hygroscopicity, phase states, and chemical properties. In this work, we employ single-particle levitation methods to analyze aerosol properties relevant to prebiotic Earth. Using a linear quadrupole electrodynamic balance (LQ-EDB) coupled with an open port sampling interface mass spectrometer (OPSI-MS), we can measure the chemical and physical changes of individual aerosol particles under controlled conditions. Single particles are levitated in the LQ-EDB for in-situ physical analysis using spectroscopy, then solubilized and aspirated via electrospray ionization into an Orbitrap mass spectrometer for molecular characterization. We investigate aerosol particles under prebiotic Earth conditions, exploring properties and chemical pathways that may have facilitated the formation of chemical precursors to life. We report the hygroscopic growth of prebiotic ocean spray aerosol to better quantify the concentration of reactive species within particles. We use mass spectrometry methods to characterize peptide bond formation in levitated particles. Earlier results have shown that aerosol particles consisting of glycine and dicyanodiamide (DCD) undergo chemistry to form diglycine when illuminated with very high intensity laser light. Here, we explore whether this chemistry occurs under light conditions that are more consistent with ambient environments on prebiotic Earth. Overall, this work examines factors such as hygroscopicity and photochemical reactivity to better understand the potential role aerosols played in the origin of life.

Adrian Huang	**Cooperative Capture of CO2 from Air with Molecular Polyamine Network Solids**	The direct air capture (DAC) of CO2 is a promising negative emissions technology that aims to offset CO2 emissions from hard-to-abate industries and address legacy emissions. While several small-scale DAC operations have been demonstrated with basic aqueous solutions or amine-functionalized solids to selectively chemisorb CO2, these technologies are limited by their low CO2 capacities and thermal energy costs (ca. 4 GJ/tCO2). One potential strategy to reduce the energy consumption associated with DAC is to design new capture materials exhibiting significantly higher sorption capacities, such that the amount of waste heat generated can be substantially reduced. In this seminar, we disclose a simple molecular triamine that rapidly captures CO2 in the solid-state when exposed to ambient air to generate a porous, crystalline ammonium carbamate network. The mechanism of this structural transformation is studied in detail using single-crystal x-ray diffraction, in situ powder x-ray diffraction, and in situ diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS). Breakthrough studies reveal that increasing relative humidity and temperature greatly improves gravimetric CO2 capacity and absorption kinetics. Specifically, under conditions reflecting a range of global temperatures and relative humidities, rapid CO2 absorption from air is observed with gravimetric CO2 capacities as high as 8.9 mmol/g, a record for any solid sorbent under DAC conditions. More broadly, these results highlight the prospect of developing a new class of tunable molecular polyamines for CO2 removal from dilute sources.

An Pham	**Unraveling Excited-State Behavior in Tetrazole Scaffolds for the Functional Design of Selective Peroxynitrite Probes**	We aim to investigate the mechanism by which tetrazole-derived fluorescent probes respond to peroxynitrite ($ONOO^-$), a highly reactive nitrogen species and key biomarker of oxidative stress. While 2,5-diaryl tetrazoles are known to undergo photolysis to form nitrile imines, the precise structure of the resulting fluorescent species and its mode of interaction with $ONOO^-$ remain poorly understood. We synthesized a tetrazole N-acylurea precursor that generates a distinct fluorescent product upon UV irradiation. This product exhibits rapid ($t_{1/2} \approx 2.3$ s), selective, and sensitive (LOD = 4 μM) fluorescence enhancement in response to $ONOO^-$, with high specificity over other reactive species. However, the photochemical transformation does not align with classic [3+2] cycloaddition pathways, and current data suggest an alternative mechanism involving stabilized nitrile imine intermediates. To clarify this, we are combining large-scale photolysis, 1D/2D NMR, and LC-MS to isolate and define the photoproduct(s) and track their reactivity with $ONOO^-$. Preliminary evidence points to a dynamic equilibrium of nitrile imine species stabilized by intramolecular hydrogen bonding or weak non-covalent interactions, which may govern the observed redox-triggered fluorescence. Transient absorbance measurements also indicate concentration-dependent speciation, further complicating mechanistic understanding. Resolving this mechanism is critical for enabling rational probe design and biological application. By elucidating the photoproduct structure and its interaction with $ONOO^-$, this work lays the foundation for future probe optimization, including improved solubility, red-shifted activation, and long-term in vivo monitoring of oxidative stress.

Bradley Kroes	**Rapid, scalable, and novel methodology for producing graphene-coated silicon microparticles**	Silicon is a promising anode material for next-generation lithium-ion batteries due to its high theoretical specific capacity (3579 mAh/g at Li15Si4) and high natural abundance, however its widespread use is still plagued by its degradation during battery cycling. The severe volumetric expansion of silicon during lithium alloy formation pulverizes the material, leading to the loss of electrical contact of the particles from the current collector and the continual growth of solid electrolyte interphase (SEI) layers on the freshly exposed surfaces of the particles. While nanostructuring silicon has proven to be an effective method to alleviate structural degradation, this route utilizes toxic chemicals and expensive manufacturing techniques, resulting in increased battery costs. Graphene coatings have also been shown to stabilize silicon anodes by providing a highly conductive and confining barrier that preserves the capacity of silicon particles, however cumbersome manufacturing techniques and the use of expensive reagents have prevented the widespread use of graphene-coated materials. Recently, our group has developed a rapid, scalable, novel, and inexpensive technique to wrap silicon particles in graphene to manufacture silicon anodes for lithium-ion batteries. This method provides an economical means to energy dense lithium-ion batteries by circumventing the need for costly materials and energy-intensive processes while still affording the increased cycling stability of silicon anodes at industrial scales. Additionally, this methodology can be extended to other electrode materials to improve their performance in rechargeable batteries.

Casey Tsai	**Modeling XFEL Experimental Design For Protein Reaction Studies Using Droplets**	Current practices in studying enzymatic reactions struggle with preserving their structure and require extra efforts to maintain their integrity. A newer technique allows for the high resolution study of protein reactions at room temperature by utilizing a drop-on-drop dispensing system with serial femto-second crystallography. This process involves a small drop of a substrate being dispensed onto a bigger microcrystal slurry droplet on a roll of tape. The merged droplet is then excited by hard X-rays, which reveals the protein structure by capturing snapshots of the reaction at intermediate reaction steps. A reaction-based diffusion model was created with Kinetiscope, a stochastic kinetic simulator, to aid in data interpretation. However, the preliminary model was not in good agreement with drop-on-drop experimental data for a model calcium-dye reaction, which prompted incorporating more realistic droplet physics into the model. The hydrodynamic calculations provide information on the initial internal structure of 2 fused droplets. . The reaction-diffusion model uses the hydrodynamic data to simulate the chemistry as a function of space and time, and visualize the distribution of the product. In parallel with improving the model, the apparatus for the drop-on-drop experiment was upgraded. The computational model is validated by newly obtained drop-on-drop experiments, proving that models have great potential to predict the chemical state of biological reactions as a function of time. Scientists can apply this ultra-fast drop-on-drop measurement system along with the model to gather more data on protein reactions and their mechanisms in realistic conditions while saving resources and energy.
Daniel Kendall	**Phenylacetaldehyde photolysis: Modeling toluene's understudied atmospheric oxidation pathway**	Atmospheric toluene oxidation can proceed through two pathways: OH-addition (90%) and H-atom abstraction (10%). The minor H-atom abstraction pathway forms a benzyl radical (PhCH2●), which then reacts with O2 to form the benzyl peroxy radical (PhCH2O2●). This minor yet significant pathway has proven challenging to study experimentally due to its relatively low branching ratio, leaving many open questions about the subsequent chemistry and impacts on atmospheric composition. Here, we use photolysis of phenylacetaldehyde (PAC) as an alternative approach to the generation of the benzyl peroxy radical. In the presence of UV light and O2, PAC forms the benzyl peroxy radical, CO, and HO2, allowing us to study toluene's H-atom abstraction pathway in isolation. PAC is introduced into an environmental chamber experiment, where it is photolyzed. Online ammonium chemical ionization time of flight mass spectrometry is used to quantify the evolution of products in real time. In addition to products consistent with known oxidation mechanisms, the initial results show the first experimental confirmation of the dimerization product dibenzyl peroxide (PhCH2O2CH2Ph) and evidence of an unknown unimolecular product. A kinetic model based on a system of ordinary differential equations is used to fit the observed time series behavior of products and provide quantification of a variety of rate constants involved in the toluene H-atom abstraction pathway.

Daniel Valenzuela	**Probing the Hot Carrier Activity and Redox Surface Properties of Gold Nanoparticles**	Gold nanoparticles have been widely used as a model system for studying how redox behavior at the nanoscale governs both photocatalytic reactivity and particle formation. I will present three distinct projects that explore different aspects of gold nanoparticle behavior, ranging from photocatalysis to redox chemistry and morphology. Although these projects address different scientific questions, collectively they illustrate the versatility of gold nanoparticles as a platform for probing surface reactivity at the nanoscale. First, I will highlight how interband and intraband excitations of gold nanoparticles provide mechanistic insight into photocatalytic processes. Our current results examining the role of hot holes in the dehalogenation of 2-iodobenzonitrile using colloidal gold nanoparticles show enhanced reaction rates under short-wavelength excitation, suggesting that interband-generated hot holes play a key role in catalyzing the rate-limiting hydride transfer step. Further experiments are underway to develop a more complete mechanistic picture. Next, I present a study evaluating the correlation between the standard redox potentials of different hole scavengers and their efficiency in hot hole quenching under interband and intraband transitions. This correlation can be useful for the optimization of the photocatalytic efficiency of the hot holes in metallic nanoparticle photocatalysis, which is overlooked compared to semiconductor-based systems. Lastly, I will introduce a prospective project that builds on our latest publication on nanoparticle redox potentials, which explores how redox potentials at gold nanoparticle surfaces influence the morphology of their growth.

Devon Stuart	**“Turn-On” Sialic Acids for Noncovalent Cell Surface Labeling**	Metabolic glycoengineering (MGE) utilizes synthetically modified carbohydrates to investigate and manipulate cellular function. Through cellular scavenging pathways, cells incorporate these sugars, modified with reactive tags like azides, into biomolecules displayed on the cell surface. Bioorthogonal reactions then allow further elaboration of these sugars with fluorescent dyes or ligands to track their expression or influence cellular interactions. However, slow reaction kinetics or chemical instability of bioorthogonal reacting partners limit MGE’s translation into complex organisms like mice. We propose a noncovalent complexation approach to MGE, leveraging the strong binding and inherent stability of binding partners in host-guest complexes. Our strategy utilizes Cucurbiturils (CB), biocompatible synthetic macrocycles that are known to bind small molecule guests with exceptionally high affinities. This system requires modifying sialic acid with a small functional group, such as trimethylsilyl amine, that would both be metabolically incorporated into the cell and have a high affinity for CB[7] (Ka = 108). Previous attempts to incorporate sugars with this cationic amine, required for high affinity binding, were unsuccessful. We anticipate that masking the amine as an azide will enable cellular incorporation. Subsequent in situ reduction to the amine will “turn-on” the affinity for CB[7] binding achieving selective labeling via noncovalent complexation. Progress toward the synthesis of multiple sialic acid analogues modified with trimethylsilyl methylazide and their incorporation efficiency are reported in this work.
Diksha Sharma	**Hydrodefluorination of Polyfluorinated Arenes Catalyzed by Iron-Complex**	Iron (II) complexes with the general formula [Fe(PP)Cl_2], containing wide-bite-angle phosphine ligands (PP) with different backbones and P- donors, and the assessment of their efficiency for the hydrodefluorination (HDF) of (poly)fluoroarenes, using HBPin as the H source, with $NaBHEt_3$ and NaOtBu as activators. Among the synthesised complexes, our results support the [Fe(Cy XantPhos)Cl_2], (Cy XantPhos = 4,5-Bis(dicyclohexylphosphino)-9,9-dimethyl-9H-xanthene) complex is the most efficient precatalyst for the process. The substrate scope for the system included hexafluorobenzene, octafluorotoluene and Decafluorobiphenyl. Mechanistic investigations revealed a distinct nature of catalysis depending on the activators employed. $NaBHEt_3$ facilitated heterogeneous catalysis, while NaOtBu promoted homogeneous catalysis, as suggested by catalyst poisoning experiments. These findings provide valuable insights into the role different activators have on the type of the catalytic process accessed: heterogenous v. homogenous. This research advances the fundamental understanding of iron(II) catalytic systems for selective C–F bond activation via HDF. The developed methodologies hold significant promise for practical applications in environmental remediation and pharmaceutical synthesis, offering chemical manipulation of fluoroarenes to either degrade these materials or enhance their value.

Elisa Olivas	**The Role of Enzyme Spatial Distribution in Enzyme Metal-Organic Frameworks using Cryogenic Electron Energy Loss Spectroscopy (cryoEELS), & Energy-Filtered TEM (EF-TEM)**	Enzyme-encapsulated metal-organic frameworks (E@MOFs) are emerging as versatile hybrid materials with applications in catalysis, biosensing, and biomedical engineering. A key challenge in advancing these materials lies in understanding the spatial distribution of enzymes within the framework and how this influences catalytic function. In this work, we present a cryogenic transmission electron microscopy (cryoTEM) approach that integrates cryogenic electron energy loss spectroscopy (cryoEELS) and energy-filtered transmission electron microscopy (EF-TEM) to visualize the elemental distribution within Urease@ZIF-8. Samples were prepared under cryogenic conditions and imaged using a Titan ETEM with a Gatan imaging filter, enabling low-dose elemental mapping of beam-sensitive systems. Elemental signals corresponding to carbon, nitrogen, oxygen, and zinc were obtained for both ZIF-8 and enzyme-loaded Urease@ZIF-8 particles. Through multivariate analysis and signal deconvolution, we resolved overlapping elemental edges and mapped the presence and localization of urease within the crystalline framework. The comparison of elemental maps from bare ZIF-8 and Urease@ZIF-8 revealed distinct distributions attributable to the enzyme, offering insight into biomolecule encapsulation and accessibility. These findings demonstrate the utility of cryoEELS and EF-TEM for probing structure–function relationships in biohybrid materials. Our approach lays the groundwork for systematic studies on enzyme spatial distribution within MOFs, ultimately aiding in the rational design of next-generation biocatalytic platforms.
Erika Chambers	**Enantioselective Alkylation of Cycloalkyl Pyridines with Chiral Lithium Amides as Traceless Auxiliaries**	Pyridine containing compounds are ubiquitous motifs among various industries, including pharmaceuticals and agrochemicals. Substituted alkyl pyridines have posed a synthetic challenge, especially in accessing them asymmetrically in part due to limitations of chiral auxiliaries. We have previously demonstrated that chiral lithium amides (CLAs), a class of non-covalent traceless auxiliaries, enable the direct asymmetric alkylation of non-enolate derived nucleophiles, utilizing 2-alkylpyridines as a model. This system provided excellent enantioselectivity for a variety of substrates and electrophiles, which is attributed to well-defined mixed aggregates formed between the lithitated alkylpyridines and the CLA. This method fell short for cycloalkyl pyridines, however, which led us to expand upon the study. It was found that use of a C2 symmetric tetraamine provides the desired substituted cycloalkyl pyridines with high enantioselectivity and generally good yields. Herein, we describe a straightforward, enantioselective method for direct alkylation of cycloalkyl pyridines, using chiral lithium amides as traceless auxiliaries, which is tolerant of a variety of activated electrophiles which can allow for further functionalization.

Esveidy Oceguera	**Efficiency of SPhos Oxidative Addition Complex (OAC-2) in Suzuki-Miyaura Cross Couplings**	One of the most important carbon-carbon bond forms in industrial and medicinal chemistry is the Suzuki-Miyaura (SM) coupling, ranking second and fifth in their respective fields according to an ACS study in 2014. Therefore the importance of more environmentally responsible methodologies pertaining to this key reaction is necessary. Current SM methodologies in micellar media do not extend to pseudohalides, such as triflates, and the less frequently referenced nonaflates. While pseudohalides expand the substrates a chemist can use, these are generally classified as polyfluoroalkyl substances (PFAs) which pose a considerable environmental concern. We herein report the use of an Oxidative Addition Complex (OAC) as a more efficient alternative to traditional mixing methods using micellar catalysis.This new methodology aims to reduce the environmental impact by utilizing fluorosulfates (R-OSO2F or R-OFs), devoid of C-F bonds as a non-PFAS alternative. This methodology supplies a diverse substrate scope that features fluorosulfates derived from naturally occurring phenols, base sensitive moieties, and moderate to high yields for couplings with late stage compounds. OAC's have a higher air stability compared to other palladium sources allowing for both the catalyst and the reaction medium to be recycled in this study after exposure to the atmosphere after extraction and still yielded high product formation in recycling study of three repetitions . This oxidative addition complex has been shown to facilitate SM couplings between aryl fluorosulfates and boronic acids with increased efficiency when it comes to palladium loading, time, reagent equivalents, and yields when juxtaposed with the current literature.

Gilad Gani	**Surface Modifications Using Reductive Desorption of Carborane Monolayers**	Self-assembly provides an affordable method for modifying surface properties, laying the foundation for many charge transport based technologies. Although current research aims to miniaturize these systems to the nanoscale, single-molecule technologies have yet to be published, and pursuing this requires a precise understanding of how to control surface structures. Recently, we studied the surface behavior of a specific class of materials, Carboranethiols, cage molecules composed of 10 Boron and 2 Carbon atoms, anchored to a metallic surface via a sulfur atom. The dipole moment in these molecules depends on the position of the carbon atoms. We observed a significant change in charge transport capabilities in aqueous solutions, influenced by the magnitude and relative orientation of the dipole moment relative to the surface. Additionally, we examined the reductive desorption behavior of the self assembled monolayers, which involves breaking the sulfur-gold bond and desorbing the molecule away from the surface. Carboranethiols with dipoles facing away from the surface showed an approximate 70 mV offset in reduction potential compared to surface-facing dipole monolayers. Finally, we measured charge transport, double-layer capacitance, and reductive desorption of carboranedithiols - molecules with two surface anchoring sulfur atoms. We believe this class of molecules is an excellent candidate for precise surface modification and could enable the development of complex atomic-scale electronic systems.
Harsh Chavda	**Indole Photocatalysts and Secondary Amine Ligands Enable Nickel Photoredox C(sp2)−Heteroatom Couplings**	Nickel-photochemical C(sp2)−heteroatom coupling reactions have emerged as a powerful tool for constructing diverse molecular architectures. However, most existing methods rely on expensive photocatalysts or specialized ligands, limiting their practicality and scalability. Here, we introduce a photocatalytic initiation strategy driven by inexpensive indoles, eliminating the need for designer photocatalysts. Additionally, we demonstrate the effectiveness of highly tunable secondary amine ligands in facilitating coupling while suppressing side reactions that sequester the Ni catalyst off-cycle. Our approach enables a broad range of amination and etherification reactions with good yields and functional group tolerance, providing a scalable platform for C−N and C−O couplings that relies on a readily available photocatalyst and cost-effective, modular ligands. Finally, mechanistic investigations suggest that the reaction operates via an unconventional aryl radical-initiated Ni(I/III) catalytic cycle, distinguishing it from traditional Ni-photoredox processes. This initiation mode, in which aryl radicals are generated under mild conditions compatible with organometallic catalysis, is expected to serve as a generalizable platform for other synthetic transformations beyond Ni-catalyzed processes.

Hashim Al Khunaizi	**Approaching the Limit: Boron Clusters as Platforms for Superhydrophobic Coatings**	Superhydrophobic coatings require incorporation of fluoroalkyl chains to minimize the surface/liquid interface interactions. However, these coatings cannot be thermally degraded and usually form surfaces with defects, that require advanced techniques to overcome these issues. In this work, we adopted a new strategy where we employ dodecaborate nanocluster supports to form densely packed fluorous materials that can be used as active components of coating materials. These clusters form defect-free superhydrophobic coating when mixed with titania in ethanol as seen by electron microscopy imaging. Specifically, the coating with perfluorobutyl functionalized cluster has an extremely low surface energy compared to the fluorous coatings reported so far. Moreover, these coatings are thermally degradable at moderate temperatures avoiding the persistence of polyflourinated substances in the environment. This work shows that these clusters can be better platforms for robust superhydrophobic coating materials and their scope can be further expanded to other coating applications.

Hernán Gómez	**Covalent inhibitors of lecithin:retinol acyltransferase (LRAT), an essential enzyme in the visual cycle**	Lecithin:retinol acyltransferase (LRAT) plays a crucial role in the visual cycle by esterifying all-trans-retinol to all-trans-retinyl esters in the retinal pigment epithelium (RPE). This study investigates the modulation of LRAT activity through synthesis and evaluation of novel halogenated compounds based on retinyl bromoacetate, a known covalent modifier of LRAT's active site Cys161 residue. We hypothesized that substituting the α-position halogen alters the electrophilicity of the inhibitor, affecting its reactivity with Cys161. A 2nd group of inhibitors was also synthesized and evaluated, comprising of retinyl esters bearing electrophilic warheads targeting cysteine residues. A series of retinyl haloacetate derivatives (fluoro-, chloro-, and iodoacetate) and inhibitors containing cysteine directed electrophilic warheads were synthesized and assessed using two assays: a recombinant glutathione-S-transferase-tagged truncated LRAT (GST-tLRAT) enzyme for quantitative IC_{50} values, and native bovine RPE microsomes to evaluate inhibition in its physiological environment. Both assays showed consistent trends. Less electronegative halogenated inhibitors showed stronger inhibition of LRAT. Inhibitors with cysteine-directed electrophilic warheads displayed similar structure–activity relationships. The RPE microsome assay yielded more robust IC50 values compared to the GST-tLRAT assay, likely due to the inhibitors' ability to penetrate the membrane where LRAT is. The GST-tLRAT assay showed similar trends and produced higher IC50 values, possibly due to solubility limitations arising from the inhibitors' hydrophobicity. These results support a structure-activity relationship from α-halogen substitution and electrophilic warhead design. The study highlights the potential for modifying electrophilic reactivity to enhance LRAT inhibition in ocular environments, opening new avenues for therapeutic interventions in visual cycle-related disorders.
Jake Stofan	**Synthesis and Reactivity of Mo Complexes Bearing the Redox-Active dppBIAN Ligand Across Several Oxidation States.**	The bis-2, 6 diisopropylphenyl acenapthenequinonediimine (dippBIAN) ligand was complexed to a Mo (IV) center in a simple ligand substitution to yield the dippBIANMoCl4 complex. The two-electron reduction in the presence of PMe3 resulted in the expected dippBIANMo(PMe3)2Cl2 complex that was characterized using NMR and XRD. Putative NMR evidence suggests an accessible tris PMe3 complex in the presence of excess ligand. Interestingly, the BIAN ligand bond distances suggests a formal 1-electron ligand reduction and a Mo (III) center. Upon another two-electron reduction, the major product was determined to be an allyl hydride complex resulting presumably from dehydrogenation and insertion of the aryl isopropyl groups of the dippBIAN ligand which was characterized via XRD and NMR. Further reactions of this allyl hydride complex with hydrogen will be discussed as well as the consequences of ligand redox-noninnocence and ancillary ligands on electronic structure.

John Saunders	**Sustainable Amination and Amidations in Continuous Plug Flow**	Reported herein is the use of a readily assembled continuous plug flow reactor used towards Pd-catalyzed aminations and with minor adjustments direct amidations of carboxylic acids. The flow system consisted of 2 syringe pumps and a peristaltic pump feeding into a PFA tubing reactor (2 mL) and out through another peristaltic pump acting as a back pressure regulator. These Buchwald-Hartwig aminations were conducted in an aqueous medium using n-propanol as co-solvent. This allowed the aqueous layer to be recycled without a reduction in yield. Additionally, the use of water avoided a buildup of insoluble inorganic salts which often leads to reactor failure. A variety of aromatic and aliphatic amines were coupled with (hetero)aryl bromides. These reactions highlight the sustainable nature due to low levels of palladium (0.5 mol %), low levels of residual palladium in products, recyclability of the reaction medium and catalyst, and low E-Factors. Using a similar reactor setup in a tandem fashion, the direct amidations of both electron-rich and -poor aromatic acids, as well as sterically hindered aliphatic acids, are efficiently coupled with a variety of amines, including the formation of Weinreb amides and peptides, in high yields. To accomplish this, the recyclable and sustainable coupling reagent, 2,2'-dipyridyldithiocarbonate (DPDTC) was used. In a 2-step manner, DPDTC produces an isolable thioester which is fed directly into the second reactor (without isolation) to react with the amine forming the desired amide. This coupling reagent is fully recyclable through a simple acid/base extraction along with the recyclable, bioderived solvent, 2-MeTHF.
Joseph Palasz	**Boiling Trees: Using Basic Organic Chemistry to Unlock Lignocellulosic Biomass**	We produce a vast quantity of plant material which is wasted every year. This material represents a compelling carbon source for chemical building blocks, materials and fuels, however we don't currently have viable processes to unlock lignocellulosic biomass effectively. Small-molecule amines are potent reagents for unravelling the structure of lignocellulosic biomass, and can be recycled using a distillation based solvent recovery scheme. This work studies the activity of simple alkylamines as pretreatment reagents for lignocellulosic biomass. The mechanism of action of the simple amines was studied using FTIR, PXRD, fluorescence Microscopy, solution and solid state NMR, elemental analysis, and through reactivity trends. This mechanistic knowledge guided the discovery of reagents which can efficiently deconstruct lignocellulosic biomass like corn stover, wheat straw, sorghum and rice straw under facile conditions.

Juancarlos Rojas	**Sustainable Catalysis: Earth abundant metals for a greener future**	As the demand for more sustainable and environmentally friendly chemical processes increase, the need to develop catalysts based on earth abundant transition metals are critical. Rare earth metals currently dominate commercial catalysis despite the high cost and environmental impact. Iron is an attractive alternative being the most earth abundant and non toxic transition metal. My work focuses on the synthesis of benchtop stable low valent iron complexes for use in catalysis. Iron pentacarbonyl, despite its ironic toxicity, serves as our source of low valent 18-electron iron. To achieve benchtop stable iron complexes we need to utilize strongly binding yet catalytically permissive ligands. Cyclopentadienones have proven effective strongly binding highly modular ligands. We make them in situ, after some work up we have our first benchtop stable iron complex. Another effective highly modular ligand type are phosphines, depending on which phosphine we could potentially tune the catalyst for different reactions. Preliminary results demonstrate activity in [2+2] cycloadditions of unactivated alkenes as well as some potential for Suzuki cross couplings. As the field progresses, building a broad robust foundation in sustainable catalysis will enable the development of more versatile and practical systems for a greener future
Julia Balsamo	**Mechanistic Insight into Intestinal α-Synuclein Aggregation in Parkinson's Disease**	Aggregation of the protein α-synuclein in the brain has been linked to Parkinson's disease development. Curiously, these aggregates appear to accumulate in the gut years prior to the onset of motor symptoms. Enteroendocrine cells may be the source of intestinal α-synuclein, as they express this protein. Enteroendocrine cells border the gut lumen; as such, they are exposed to the gut microbiota and its metabolites. Interestingly, these cells also synapse with vagal neurons, which innervate the gut and brain. Through this connection, Parkinson's disease pathology may originate in the gut and spread to the brain. Unfortunately, effective therapeutics are lacking due to a limited understanding of the mechanism by which intestinal α-synuclein aggregates. Our work helped elucidate a gut bacterial metabolic pathway responsible for this aggregation event. As demonstrated in bacterial cultures and in enteroendocrine cells, a cascade of oxidation reactions that results in α-synuclein aggregation is induced upon respiration of the oxidant nitrite by Enterobacteriaceae. In further studies, we observed that manipulating intracellular dopamine concentration in enteroendocrine cells allows for some control of α-synuclein aggregate formation. Our understanding of this dopamine-dependent pathway has enabled us to discover dietary molecules that significantly limit α-synuclein aggregation. These results are critical to revealing new avenues for targeted therapeutics to treat Parkinson's disease, enabling us to mitigate α-synuclein aggregate formation in the gut before neurodegeneration in the brain may occur.

Kam Tung Chan	**Nitrate Photolysis in Solution from First Principles Molecular Dynamics and Machine Learning**	Nitrate anion in aerosol particles is an essential sink of nitrogen oxide species (NOx). Its photodissociation is a 'renoxification' process, which converts nitrate anion solvated in water or deposited on surfaces back into NOx to the atmosphere. The dissociation of nitrate anion at its triplet state can follow two channels: (1) nitrogen dioxide and oxygen anion radical; (2) nitrite and oxygen atom. Despite the well-studied macroscopic kinetics, the microscopic details of the two channels and the connection to reaction rates are still inconclusive. Experiments have shown that nitrate photodissociation in aqueous solutions has a low quantum yield of ~ 1%, whereas it is 100% in the gas phase. Here, we employ excited-state ab initio metadynamics simulations to explore the complex free energy landscape of nitrate photolysis in water and reveal the molecular origin of its low quantum yield. Our simulations reveal a metastable solvation cage complex that allows the photo fragments to recombine or deactivate through non-radiative processes. The molecular details of the two reaction paths probed in our simulations also explain the different temperature dependence of their quantum yields observed in experiments. A reactive machine-learning potential fitted to the ab initio metadynamics allows us to obtain accurate rates in water at various temperatures, thus providing a fundamental understanding of a key process of the nitrogen cycle in the environment.
Katia Hatem	**Direct Measurements of Criegee Intermediates Using Cavity Ringdown Spectroscopy for the Ozonolysis of a Series of C6 Alkenes**	Ozonolysis of alkenes via non-photolytic pathways is a significant oxidation reaction that occurs in the troposphere, contributing to the formation of highly reactive species such as hydroxyl (OH) radicals and Criegee Intermediates (CIs). In this study, the ozonolysis of 1-hexene and its C6 isomers (2-ethyl-1-butene, 2,3-dimethyl-1-butene, 2-methyl-1-pentene, 3,3-dimethyl-1-butene, 3-methyl-1-pentene, and 4-methyl-1-pentene) was investigated to quantify the yield and stabilization fraction of the C_1 Criegee Intermediate, CH2OO. Measurements were conducted at room temperature using ultraviolet cavity ringdown spectroscopy (UV-CRDS) over the 378–387 nm range at 7 Torr, with reaction times varying from 0.2 to 0.8 seconds and variable ozone/alkene concentrations. The yield of C1 Criegee Intermediate was evaluated by simulating the production reactions of the Criegee Intermediate with different branching ratios, utilizing Kintecus software for kinetic modeling. Quantification of the stabilized Criegee Intermediate (sCI), along with C□-specific intermediates, enabled a detailed evaluation of how alkene structure influences product distribution and stabilization. Results show that branching closer to the α-carbon increases the stabilization fraction of the C1 Criegee Intermediate, while further branching leads to reduced stabilization. This trend suggests that proximal branching enhances energy loss from the intermediate, thereby promoting stabilization. Systematically varying the branching of alkenes provides knowledge into the chemical reactivity and its effects on the yield. These measurements provide a detailed reaction network, offering insights into the underlying mechanism allowing for improved predictive models.

Lilian Zeinalvand	**Understanding the Structure and Dynamics of Peptide-Based Coacervates with In-Situ Liquid and Cryo-TEM**	Coacervates play a critical role in fields ranging from biomaterials to cellular organization. Among these, peptide-based coacervates are particularly compelling due to their relevance as fundamental biological building blocks. But life exists far from equilibrium, and many biological structures are maintained only through constant energy input. Inspired by this, chemists have developed dissipative systems in which structure is dynamically assembled and disassembled through coupled chemical reactions. These systems give rise to materials with unique structures and behaviors that differ from their equilibrium counterparts. In this study, we investigate disulfide-linked peptide coacervates, comparing two modes of formation: a stable, pH-driven pathway and a nonequilibrium dissipative pathway. While coacervates are commonly studied using optical microscopy, their nanoscale structure and dynamics remain underexplored. To address this, we use liquid-phase transmission electron microscopy (LPTEM) to directly observe coacervate formation in real time, complemented by cryogenic TEM to confirm and expand our structural insights. Our electron microscopy findings provide critical insights into nanoscale coacervate formation mechanisms highlight how dynamic interfaces and non-equilibrium processes reshape our understanding of peptide-based condensates with broader implications for designing biomimetic materials and understanding protocellular systems.
Linus Murphy	**Simulation Development for HgTe Quantum Dot Growth**	HgTe Quantum Dots (QDs) have demonstrated potential in fields such as optoelectronics and bio-imaging due to their highly tunable band gap, especially in the short-wave infrared range. The full realization of this applicability is currently hindered by an inability to consistently produce QDs of desired sizes, as the mechanisms governing crystal growth are not well understood. Other QD systems have been known to follow both Ostwald Ripening and Size Focusing growth mechanisms via Small Angle X-ray Scattering, but there has yet to be a comprehensive study of QD growth extrapolating size distribution from QD spectra. We have developed a kinetic Monte Carlo simulation of QD crystal growth, allowing for variability in injection speed, size dependance, and monomer size.

Luke Jackson	**Carborane Ligated Iridium Hydride Cluster Enables Recyclable Solution Phase Crabtree Type Hydrogenation**	Iridium is widely used in homogeneous hydrogenation, yet its most prominent example, (Ir(COD)(PCy3)(py))(PF6) (Crabtree's catalyst), deactivates after a single recycle by clustering into a hydride-bridged trimer. Current strategies to improve recyclability rely on MOF immobilization or bulky weakly coordinating anions, but these still demand high H2 pressure or solid supports, leaving a truly recyclable low-pressure homogeneous system elusive. We now introduce the first fully solution-phase, recyclable Crabtree-type catalyst, produced by coupling a phosphino-perchlorinated carborate anion with an iridium precursor to yield Ir(COD)(PiPr2CB9Cl9). Hydrogenation of this complex produces an orange precipitate identified as an hydride-bridged trimer. Although its full structure is under further study, addition of a donor such as THF converts the trimer into the catalytically active $IrH_2(PiPr_2CB_9Cl_9)(THF)_2$. Rigorous testing shows that the catalyst efficiently hydrogenates primary, secondary, tertiary, and tetrasubstituted alkenes. On cyclohexene in CH2Cl2, it retains roughly one-third of its initial rate through five cycles when a modest dose of THF is added, a measure that likely suppresses late-stage trimerization as alkene is depleted, roughly doubling the second-half reaction rate compared with THF-free runs and delivering the first truly recyclable solution-phase Crabtree analogue.
Madison Esposito	**Low-valent metal-organic materials with group 9 metals and phosphine ligands**	Metal-organic frameworks (MOFs) are crystalline, porous materials often formed by combining hard Lewis acidic high-valent metal ions (e.g. Zr(IV), Zn(II), etc.) with hard Lewis basic ligands (e.g. carboxylates, imidazolates, etc.). MOFs have been studied for their applications in gas storage, separations, heterogeneous catalysis, and other processes. Low-valent metal-organic frameworks (LVMOFs) are similar self-assembled materials containing metal ions in the (0) or (+1) oxidation states (soft Lewis acidic metals); many prevalent homogeneous catalysts contain these highly active low-valent metals. By incorporating low-valent metals into extended networks, LVMOFs and related materials may serve as a bridge between the reactivity of homogeneous catalysts and the ease and recyclability of heterogeneous catalysts for small molecule transformations. The Cohen Lab has pioneered the development of low-valent metal-organic materials from Pd(0), Pt(0), Rh(I), and Ir(I) precursors using tetratopic phosphine linkers (soft Lewis basic ligands). Herein, we report recent discoveries in the synthesis, characterization, and catalytic properties of materials synthesized from Rh(I), Ir(I), and Co(II) precursors with tetratopic phosphine linkers. Future studies will utilize a greater diversity of phosphine ligands and metal precursors, and novel materials will be applied in a wider range of catalytic transformations.

Marvin Santiago	**Degradable poly(N-vinylpyrrolidone) synthesis in water: advancing green polymer chemistry**	Many efforts have been made to address the problem of plastic pollution, including the development of polymers that are degradable from the time of their production. A popular method for achieving this with vinyl polymers is the radical copolymerization of their monomers with small molecules that introduce labile bonds to the polymer backbone. This technique depends on matching the radical reactivities of the two comonomers to ensure a random distribution of these labile bonds. The high radical reactivity of less activated monomers, a type of vinyl monomer with weaker inductive radical stabilization, makes their incorporation into degradable polymers challenging, and there are few examples of these copolymers in the literature. This is especially relevant because N-vinylpyrrolidone, a less activated monomer, is a commercially important polymer that is both synthesized and used in water, leading to the accumulation of poly(N-vinylpyrrolidone) in waterways. Here, water-soluble copolymers of N-vinylpyrrolidone were synthesized using a highly scalable monomer that introduces disulfide bonds along the polymer backbone. Molecular analysis enabled the probing of detailed sequencing along the backbone and revealed the random incorporation of both monomers. Through derivatization, this monomer became water-soluble and enabled the aqueous synthesis of degradable polymers with high molecular weights, and eliminated the need for organic solvents. Under reducing conditions, these polymers broke down into low-molecular-weight oligomers. Thus, a circular process of synthesis, use, and degradation of poly(N-vinylpyrrolidone) in water has been established.

Md Shaihan Bin Iqbal	**Photochemically enhanced burn rate of solid propellant**	The control and enhancement of burn rates in solid propellants are critical for improving performance, safety, and adaptability in propulsion systems. This study investigates the photochemical enhancement of burn rates in nitrocellulose (NC)-based solid propellants doped with the photochromic molecules 2-chlorohexaarylbiimidazole (o-Cl-HABI), spiropyran, and diarylethene. Upon UV irradiation (365 nm), only the HABI molecules generate reactive lophyl radicals, significantly enhancing combustion by approximately 400% through catalytic reaction pathways. Electron paramagnetic resonance (EPR) measurements conclusively demonstrate the formation and sustained presence of lophyl radicals within irradiated samples. Systematic combustion tests reveal that varying the concentration of o-Cl-HABI from 0.001 M to 0.1 M effectively tunes the burn rate, with optimal doping concentrations identified to achieve maximum combustion efficiency. Differential scanning calorimetry (DSC) measurements indicate unchanged thermodynamic behavior, with similar decomposition temperatures observed for both undoped and doped systems, highlighting that the enhancement mechanism is predominantly kinetic rather than thermodynamic. High-speed imaging further confirms that UV irradiation significantly reduces ignition delay times and markedly increases flame propagation velocities. This photochemically triggered radical formation introduces an innovative approach to real-time combustion modulation, potentially enabling precise, on-demand propulsion control in aerospace and defense applications. The findings presented here offer valuable insights into radical-mediated combustion enhancement mechanisms, paving the way for the development of advanced, controllable, and high-performance energetic materials.
Min Kyu Lee	**Development of Biodegradable Thermoplastic Elastomers for Single-Use Medical Devices: A Sustainable Alternative to Conventional Polymer**	The U.S. healthcare sector generates millions of tons of plastic waste annually, with single-use devices such as catheters contributing significantly to environmental pollution. Intermittent urinary catheters alone have been estimated to create up to 85 million pounds of waste annually in the US. This project explores the development of biodegradable, medical-grade thermoplastic elastomers to replace conventional polymers like PVC and silicone. A novel formulation using poly(butylene adipate-co-terephthalate) (PBAT) blended with triethyl citrate (TEC) was optimized for flexibility and durability, targeting compliance with ASTM standards for single-use intermittent urinary catheters. Material characterization (FTIR, TGA, DSC, Instron) confirmed the mechanical and thermal viability. A provisional patent was filed, and preclinical pathways, including FDA 510(k) approval and SBIR resubmission, are underway. Future efforts focus on biodegradability testing to solidify the overall characterization of the material and produce a stronger profile in possibly replacing PVC and silicone in medical-grade applications.

Nathan Coddington	**Nickel-Catalyzed C-CN Coupling of Benzonitriles and Cyclopropyl Ketones**	The synthesis of nitrile-containing compounds often requires the use of hydrogen cyanide, cyanide salts, or other toxic cyanide sources. Benzonitriles are ideal cyanating agents due to their modest toxicity; however, their chemical robustness makes them challenging coupling partners. Herein we describe a nickel-catalyzed ring opening and cyanation of cyclopropyl ketones using a comparatively non-toxic benzonitrile as the cyanide source. We demonstrate moderate functional group tolerance and modest to good yields. Furthermore, stoicheometric nickel complex experiments and kinetic measurements suggest the identity of the active cyanide source to be in-situ generated trimethylsilyl cyanide. We hope this work broadens the scope of cyanation reactions and lays the foundation for future reactions that use benzonitriles as non-toxic cyanating reagents.
Nehal Idris	**Understanding the Encapsulation Behavior of Nile Red within Nonionic Block Copolymer Coacervates and Sefl-assembled Particles**	The encapsulation of small molecules in nonionic block copolymer coacervates holds significant potential across many fields. However, the mechanism driving this process remains largely unexplored. Here, we investigate the partitioning behavior of the hydrophobic dye Nile red in two nonionic block copolymer systems: Polyethylene glycol-block-polymethyl methacrylate (PEG45-b-PMMA) and polyethylene glycol-block-polycaprolactone (PEG45-b-PCL). We employed Confocal Laser Scanning Microscopy to quantify partition coefficients as a function of degree of polymerization (DP) of the PMMA block, dye concentration, and water. Our results show that the partition coefficient increases with PMMA DP and water content. These results show that the relative solubility between the dilute and dense phases plays a dominant role in partitioning.

Parian Poorjafari Jafroodi	**Evaluating Hole Scavenging Efficiency in Metal Nanoparticle Photocatalysis**	Photocatalysis on metal nanoparticles has garnered recent attention due to their ability to generate energetic charge carriers under light irradiation. Especially, metal nanoparticles can generate hot holes with comparable oxidation potentials. In this study, we investigate the power of these potentials by correlating their efficiency of quenching some typical hole scavengers with the standard redox potentials of these hole scavengers. As a result, establishing this correlation will allow us to precisely assess the photocatalytic efficiency of the hot holes and will provide deeper insight into optimizing hot hole utilization in plasmonic photocatalysis. Methanol, ethanol, ascorbic acid, and sodium sulfite—chosen for their well-characterized redox potentials—are served as hole scavengers. Their standard reduction potentials (vs. SHE) are converted into absolute vacuum energy levels to be better compared to the energy levels of hot holes. Colloidal metal nanoparticles in aqueous solutions containing these scavengers are photoexcited under LED irradiation in nitrogen atmospheres to prevent electron scavenging by O_2. Oxidized products are quantified using gas chromatography and nuclear magnetic resonance, then the hole scavenging efficiency is determined through quantum yield measurements of the entire oxidizing process.
Partho Paul	**Redox Potential Modulation of Quinones via Intramolecular Hydrogen Bonding for CO_2 Capture applications**	Tuning the redox properties of quinones is central to optimizing their performance in electrochemically driven CO_2 capture systems. While intermolecular hydrogen bonding with alcohol additives is known to influence quinone electrochemistry, the effect of intramolecular hydrogen bonds—where the donor is covalently tethered to the quinone core—remains underexplored. Here, we present a systematic study of how intramolecular hydrogen bonding motifs modulate quinone redox potentials, with a focus on designing molecules that favor CO_2 capture at milder applied voltages. Using a series of hydroxymethyl benzoquinones and napthoquinones, we observe significant anodic shifts in reduction potentials, in some cases exceeding 200 mV relative to unsubstituted analogs. These shifts are attributed to stabilization of the reduced quinone anion via internal H-bonding, supported by electrochemical analysis and spectroscopic characterization. Complementary trends in substituent effects reveal the importance of both electronic and steric factors in tuning redox behavior. Our findings establish intramolecular hydrogen bonding as a powerful and modular handle for modulating quinone electrochemistry and offer design principles for next-generation CO_2 capture agents.

Pauline Bianchi	**How subtle interactions drive selectivity in intramolecular cyclizations: A computational insight**	Intramolecular cyclizations often rely on fine energetic differences between competitive transition states, influenced by substituent effects or non-covalent interactions. Understanding what drives chemo-, regio- and stereoselectivity in such cases remains challenging, but can already be rationalized using advanced computational tools. In this work, we highlight two distinct, yet conceptually related case studies where selectivity arises from subtle transition state (TS) stabilization, investigated in silico. The first study focuses on an α/β hydrolase that catalyzes a double anti-Baldwin cyclization, forming a fused 6-7 bicyclic ether. Molecular dynamics simulations and MM-GBSA analysis allowed us to identify a non-canonical catalytic tetrad (Ser170, His169, Asp314, Asn342) and show how electrostatic interactions with the ligand drive both regioselectivity and overall reactivity, in line with mutational studies. In the second case, we investigate a rare [8+2] intramolecular cycloaddition forming stereodefined hydroazulenes. DFT calculations highlight how small conformational changes and substituent effects govern the relative TS energies, and how these match the observed selectivities. Together, these two examples illustrate how a detailed computational approach can reveal the non-intuitive and subtle interactions behind complex selectivity patterns, providing insights that are transferable to both enzymatic and synthetic systems.
Pedro De Allende	**Exploring the Optical Properties of Brown Carbon Aerosol Using Single Particle Levitation**	Aerosol particles are central to atmospheric processes, with significant effects on climate, air quality, and human health. Their ability to scatter and absorb radiation, serve as cloud condensation nuclei, and participate in multiphase chemical reactions makes them important components of the atmosphere. The radiative impact of aerosol particles is highly dependent on their chemical composition, determined by their source, and physical properties. Aerosol particles may be directly emitted (primary aerosol) or formed by the condensation of organic vapors (secondary organic aerosol, SOA). A component of SOA, brown carbon (BrC) has been shown to be light absorbing in the visible region of the solar spectrum. BrC is primarily produced from biomass burning and fossil fuel combustion due to direct emission and secondary chemistry in the smoke plume. An improved understanding of the physicochemical properties that regulate the impact of BrC in the atmosphere is necessary to constrain their atmospheric lifetime, understand their interactions with clouds, and assess their overall radiative effects. In this work, we use a linear quadrupole electrodynamic balance (LQ-EDB) to levitate single or multiple aerosol particles under controlled atmospheric conditions. We will use an elastic light scattering method, Mie resonance spectroscopy, to determine the size and optical properties of our samples, described by the scattering and absorbing parts of the refractive index. We will characterize the optical properties of various aqueous BrC species as a function of environmental conditions and particle pH, including nitrophenols (NP), phenolic acids, and imidazoles, and explore how chemical transformations evolve the optical properties.

Piyusha Lotlikar	**Exploration of the photochemistry of Ru(II) complexes with bidentate S donors**	Ruthenium polypyridyl complexes are widely used scaffolds for photoactivated chemotherapy and photodynamic therapy in the treatment of cancers due to beneficial photochemical and photophysical properties. Their favorable photochemical reactivity can also be leveraged for the release of bioactive ligands that imbue further functionality to the complex, for example a chemotherapeutic or other such pharmacologic. In this work, we devised a series of bis-bipyridine ruthenium complexes with a well-established hydrogen sulfide (H2S) donor ligand, GYY4137, bound in bidentate fashion. Designed to significantly dampen the kinetics of photochemical ligand release and afford greater temporal resolution to H2S, we instead observe interesting bipyridine ligand loss following a period of blue light irradiation. Across the series of compounds, we observe similar reactivity and map trends therein against the chemical properties of the ancillary bipyridine ligands. We further employ density functional theory to justify the observed reactivity in the context of other similar ruthenium polypyridyl complexes.
Preeta Pratakshya	**Backbone-modified proteins as functional biomaterials**	Amphiphilic proteins and peptides offer a unique combination of design modularity and chemical versatility, enabling them to spontaneously assemble into dynamic, stimuli-responsive nanostructures. Their tunable architecture and ease of functionalization make them exceptionally well-suited for creating adaptive, biocompatible materials with diverse applications, including therapeutics, drug delivery, sustainability. Here, we present a novel strategy for engineering amphiphilic proteins through direct backbone modification, providing a new way to tune their assembly and function. Inspired by natural products such as RiPPs, our approach enables precise control over protein amphiphilicity in a way that differs from conventional side-chain engineering methods. We demonstrate that these backbone-modified proteins can self-assemble into functional nanostructures capable of encapsulating hydrophobic molecules that are otherwise insoluble in water, highlighting their potential as biosurfactants and drug delivery vehicles. Overall, our work provides a new platform for designing self-assembling proteins with broad potential as functional biomaterials.

Rajib Mandal	**New-to-Nature Hydrogenases for the Asymmetric Reduction of Unactivated Olefins**	Reduction of carbon–carbon double bonds is a fundamental transformation in synthetic chemistry, industry, and biochemistry. Synthetic chemists and nature have evolved distinct strategies to accomplish this reaction. In biology, olefin reduction proceeds via hydride equivalents delivered by cofactors such as FADH2 or NAD(P)H. This mechanism restricts enzymatic reductions to electron-deficient alkenes, like α,β-unsaturated carbonyls. Enzymes capable of reducing isolated, unactivated olefins are exceedingly rare and rely on similar hydride-based pathways. In contrast, synthetic chemists have developed diverse hydrogenation strategies, most commonly using hydrogen gas and transition-metal catalysts (e.g., Pd, Pt, Ir)—a reactivity mode inaccessible to biology. While synthetic methods offer broad utility, enzymatic olefin reduction has inspired new catalytic approaches, particularly for highly enantioselective hydrogenations. Achieving precise spatial control over hydrogen delivery—the smallest reactive group in chemistry—is inherently challenging, and asymmetric hydrogenation has long fascinated synthetic chemists. High enantioselectivity is typically achieved for electron-deficient alkenes that support organized, chelation-stabilized transition states. Although Ir-catalyzed systems with chiral P,N-ligands have expanded the scope to some non-coordinating alkenes, asymmetric reduction of unbiased, unactivated olefins remains difficult. Here, we report engineered proteins that catalyze asymmetric reduction of isolated, unbiased olefins via a radical-based hydrogenation mechanism unprecedented in biology. These new-to-nature enzymes display broad scope, including substrates that are challenging for small-molecule catalysts. Promiscuous and highly stereoselective, these enzymes introduce a fundamentally new biochemical logic for olefin reduction and provide a platform for next-generation biocatalytic hydrogenation.

Riya Singh	**Polymerization-Induced Condensation (PICON)**	Biomolecular condensates compartmentalize reactions within the crowded cellular environment, often enhancing biochemical processes by locally concentrating reactants. While it's widely assumed that condensates accelerate reactions by increasing local concentrations, recent studies show their influence on reaction kinetics is not always straightforward, they can speed up, slow down, or have no effect depending on the molecular context. Despite their central role in cellular organization, the dynamic relationship between condensate state and reaction kinetics remains poorly understood. Here, we introduce a polymerization-induced condensation (PICON) system as a synthetic model to probe how condensate formation influences reaction kinetics. Our system employs photo-initiated RAFT polymerization of a diblock copolymer to drive polymer growth and condensate formation simultaneously, mimicking how intracellular condensates form through phase separation during ongoing biochemical reactions. We observe two distinct transitions: the formation of liquid-like condensates, followed by their transformation into dynamically arrested gel phase. Interestingly, the polymerization proceeds at a steady rate during the initial liquid phase, but speeds up significantly as the system transitions into a gel-like state. This increase in rate is likely driven by shifts in the condensate's internal dynamics and material structure. Overall, this study provides insight into how the evolving state of condensates can regulate reaction kinetics, offering a synthetic framework to explore principles relevant to intracellular organization and function.
Samantha Ono	**Development of Surface-Enhanced Raman Probes for the Detection of Heterogeneous Disease Biomarkers**	Early and accurate disease diagnosis is crucial for effective treatment and improved patient outcomes. The extreme heterogeneity in composition and temporospatial arrangement of molecules within diseased tissues makes diagnosis and prognosis challenging when relying on individual biomarkers. The rapid and accurate detection of multiple biomarkers in single samples is therefore of utmost clinical importance. Surface-enhanced Raman spectroscopy (SERS) is an exceptional platform for potential multiplexed biomarker detection methods due to its sharp, narrow spectral bands, high signal, and simultaneous excitation of multiple analytes from one laser channel. However, a major limitation is the scarcity of spectrally distinct reporter molecules, or "tags" for SERS probes that do not overlap with endogenous biomolecules. To address this challenge, we are developing a modular library of polyyne-containing small molecules as SERS tags. Alkynes generate Raman signals in the biologically silent spectral region, and increasing polyyne chain length systematically red-shifts the Raman signal, enabling multiplexed detection within this window. We optimized a robust synthetic platform to overcome the notorious instability and poor solubility of polyynes to produce multi-functional Raman tags. We also investigated how chemical functionalization influences Raman shift frequencies to generate unique spectral signatures. This work expands the chemical space of Raman reporter molecules, facilitating simultaneous detection of multiple biomarkers for enhanced disease diagnosis.

Sara Murphy	**Effects of Functional Groups on Product Distributions in RO2 + RO2 Reactions**	The peroxy radical (RO2) self-reaction has recently been the subject of significant study, as the importance of several gas-phase reactions pathways have been reevaluated or discovered. Studies of high RO2 reaction systems have also demonstrated the significant effects of functionalization on peroxy radical fate, with the branching to different reaction pathways and products changing significantly with differing functionalization. In this work, we examine the effect of functionalization on product distribution in a variety of high RO2 systems. By photolyzing organic iodides corresponding to the peroxy radicals of interest in a small environmental chamber, we produce these peroxy radicals directly to achieve high concentrations of RO2 and isomeric specificity and detect the resulting products with ammonium high resolution chemical ionization mass spectrometry (CIMS). Using the chemical formulas of the resulting products, we determine the fraction of these products that are consistent with fragmentation, dimerization, and radical termination reactions, and compare these metrics for the reactions RO2 with a variety of functional groups.
Shruti Jain	**Photovoltage of BiVO4 Photoelectrode Junctions from Applied Bias Vibrating Kelvin Probe Measurements**	Photoelectrochemical cells (PECs) can produce hydrogen fuel via solar water splitting, but efficiencies for most semiconductor electrodes are low due to poor junctions formed at the semiconductor-liquid interface. Here, we use Vibrating Kelvin Probe Surface Photovoltage Spectroscopy (VKP-SPS) as a contactless and non-invasive tool to characterize the photoelectrochemical performance of BiVO4 photoanodes as a function of the illumination, wavelength, light intensity, and applied bias. We focus on Bismuth Vanadate ($BiVO_4$) water oxidation photoanodes because of their favorable optical bandgap (2.4eV), chemical stability, and relatively high activity. It has been hypothesized that the BiVO4–liquid junction becomes more rectifying under an applied bias greater than 0.6 V vs RHE, resulting in a higher photovoltage outcome. Therefore, it is believed that an understanding of the relation between applied bias and photovoltage can benefit the search for solid-liquid junctions with enhanced energy conversion capabilities. Overall, the insights from VKP-SPS measurements aim to elucidate the charge transfer processes in BiVO4 to enhance PEC efficiency for solar fuel production.

Silvia Rivera	**Diversity-oriented photobiocatalytic synthesis via stereoselective three-component radical coupling**	Enzymatic multicomponent C–C bond forming reactions suitable for diversity-oriented synthesis remain rare. Using cooperative photobiocatalysis, we developed a stereoselective three-component radical C–C coupling process which is not previously known in either organic chemistry or biochemistry. The repurposing and directed evolution of C–C bond forming pyridoxal decarboxylases enabled variability in all three coupling fragments, giving rise to six classes of valuable products for diversity-oriented synthesis. These encompass non-canonical amino acids, cyclic amidines, unnatural pyroglutamic acids, unnatural prolines, bicyclic amino acids and disubstituted carbonyls, many of which are nontrivial to prepare by other chemical or biocatalytic methods even in racemic form. This photobiocatalytic platform integrates a range of asymmetric catalysis concepts, including remote stereocenter construction, stereodivergent catalysis, kinetic resolution and parallel kinetic resolution, achieving excellent enzymatic diastereo- and enantiocontrol over radical intermediates eluding synthetic catalyst systems. Furthermore, the broad scope and complementary activity of evolved enzyme variants allowed combinatorial library synthesis with excellent efficiency, facilitating the generation of structurally and stereochemically diverse molecular scaffolds for medicinal chemistry research.
Srijita Pal	**Probing the surface chemistry of porous materials with reactive organic dyes**	Modification of the external surface of porous materials like Metal-Organic Frameworks (MOFs) and Covalent-Organic Frameworks (COFs) plays a critical role in understanding the nucleation and growth of these extended frameworks, as well as their interactions with other molecules that are important for the preparation of composite materials. Despite the great interest in these compounds, the surface chemistry of these materials is still not well understood. BODIPY dyes having different functional groups can be used to investigate the surface chemistry of these porous materials. BODIPY dyes with aldehyde (BODIPY-CHO) or amine (BODIPY-NH2) functional group can be used to probe the presence of unreacted terminal groups at the surface/edges of imine-based COFs. COFs will react with BODIPY-NH2 or BODIPY-CHO, depending on the surface/edge termination and this can be quantified using UV-Vis and fluorescence spectroscopy. Similarly, BODIPY dyes with carboxylic acid (BODIPY-COOH) and amine (BODIPY-NH2) functional group can be used to address different facets in anisotropic MOFs like DMOF-1, which has four faces terminated by Zn-carboxylate bonds, and two faces terminated by Zn-amine bonds. BODIPY-COOH and BODIPY-NH2 can be selectively immobilized on the carboxylate terminated face and amine terminated face of the MOF crystal respectively and this can be imaged using confocal microscopy. Coordinating dyes like BODIPY-COOH can also be used to evaluate the accessibility of the metal nodes in MOF-polymer composite materials like mixed-matrix membranes (MMMs). The results of the use of these dyes as probes for COF and MOF surfaces will be presented.

Takashi Kaneko	**Radical-Free Digital Light Processing of Hydrogels via Photo-Caged Cyclopentadiene Diels–Alder Click Chemistry**	Light-controlled chemistries have transformed 3D printing and microfabrication by enabling spatial and temporal precision in material patterning, particularly for soft materials used in biomedical applications. Synthetic hydrogels that emulate the extracellular matrix are foundational in areas such as 3D cell culture, therapeutic delivery, and soft robotics. While digital light processing (DLP) has emerged as a powerful platform for high-resolution hydrogel printing, conventional systems typically rely on radical-mediated photopolymerization. These reactions, though efficient, can degrade sensitive biomolecules and limit downstream chemical modifications due to the uncontrolled nature of radical species. In this work, we report a radical-free DLP strategy using aqueous photoresins based on a Diels–Alder click chemistry between photo-caged cyclopentadiene (Cp) and maleimide. Upon 365 nm irradiation, Cp is efficiently uncaged and undergoes rapid cycloaddition with maleimide partners, forming covalent networks with high efficiency. The two-component resin system enables tunable mechanical properties and supports the fabrication of submillimeter-scale features with high fidelity. Notably, unreacted functional groups remain accessible after printing, allowing for post-fabrication spatial patterning of small molecules entirely free of radical involvement. This chemically orthogonal, biocompatible approach provides a new class of photoresins for 3D printing that overcome limitations of radical-based systems. It holds broad promise for constructing adaptive soft materials, architected biomaterials, and 4D-printed systems where precise control over chemical composition and functionalization is essential.
Tianren Zhang	**Expanding the Scope of NASICONs to Ammonium Transition Metal Diphosphates**	Few researches have been done on the solid state ionic conductivity of ammonium transition metal diphosphates, which are structurally similar to NASICONs. This work explores the potential of ammonium transition metal diphosphates with the formula of NH4MP2O7 as a new class of superionic conductors, with M being Sc, Al, Ga, V, and Y. The synthesis is carried out by direct sintering at low temperatures and washing with DI water. The structure is characterized by powder XRD and solid state NMR, and the conductivity is measured by electrical impedance spectroscopy. Results show that the proposed phases are valid with good purity, and that the structure could accomodate a wide spectrum of transition metals with drastically different lattice volumes. Solid state conductivity is measured to be comparable to those of contemporary NASICONs with the merit of easy synthesis and air stability. This work indicates that NH4MP2O7 is a promising candidate for solid state electrolytes in batteries or other electrochemical devices. Further work is necessary to explore the optimized environment to achieve the maximum conductivity.

Timothy Chau	**Computational Study of Water's Effect on Isoprene-Derived Peroxy Radical Hydrogen Shift Reactions**	Volatile organic compounds (VOCs) are emitted into the atmosphere from a variety of anthropogenic and natural sources. Once emitted, they undergo oxidation. This plays a key role in important atmospheric processes including secondary organic aerosol and ozone formation. Water vapor is one of the most abundant minor constituents of the atmosphere, but its impact on VOC oxidation remains understudied, due in part to technical challenges with its introduction into atmospheric oxidation experiments. In previous work, there has been limited evidence that water may catalyze the unimolecular and self-reactions of peroxy radicals (RO2), which are a key intermediate in VOC oxidation. Here, we computationally examine interactions between water and peroxy radicals derived from isoprene oxidation, which is well-understood under dry conditions, and is one of the most abundant non-methane VOC. More specifically, we aim to understand how water perturbs the kinetics of intramolecular hydrogen shifts of various conformers of isoprene-derived peroxy radicals. Using density functional theory (DFT) calculations, we determined the optimized geometries and frequencies of RO2 radicals and RO2-H2O complexes. We then used DLPNO-CCSD(T) calculations to obtain barrier heights of the reactions. Rate coefficients were calculated using multi-conformer transition state theory (MC-TST) and compare well with previously reported results. A similar approach was used to calculate rates for hydrogen shifts of RO2-H2O complexes. The results provide insight into how water can affect oxidation mechanisms and kinetics of VOCs, and will inform the design and interpretation of environmental chamber experiments focused on probing the role of water in isoprene oxidation.
Tommy Frisch	**Renewable and Biodegradable Polyurethanes as Alternatives for Commercial Plastics**	The devastating environmental consequences of plastic production and waste are undeniable. Each year, over half a billion tons of plastic are produced from petroleum-sourced materials. On every continent and in every ocean, plastic pollution destroys ecosystems. Sustainable alternatives for current practices in the plastic industry are needed. Polyurethanes, which account for 10% of global plastic production, are a versatile class of plastic made up of two major components. Variation in these components, polyol and diisocyanate, have a dramatic effect on the properties of polyurethanes. The vast majority of polyurethanes are produced with the use of aromatic diisocyanates, which have not been shown to be renewably sourced. In this project, polyester polyols composed of synthetic algae-based monomers were utilized to produce 100% renewable and biodegradable polyurethanes with aliphatic diisocyanates. In subsequent studies of aromatic and aliphatic components of polyurethanes, high performance sustainable alternatives were developed for a wide range of polyurethane applications. These alternatives display mechanical and thermal properties that rival commercial standards, along with excellent rates of biodegradation. This work suggests that commercial polyurethanes can be reengineered for renewability and biodegradability.

Tyler Kerr	**A Highly Crystalline Dodecaborate Radical?**	Radical anions of persubstituted dodecaborate clusters (B12X121- X = alkoxyl, benzoxyl, methyl, halogen) have been isolated, and electrochemical studies have shown very large differences between the reduction potentials of electronically similar compounds. Most of the examples that have been well-characterized have the empirical formula B12(OR)12n- where R is alkyl or benzyl. To date, only one report of the radical anion-containing compound, CsB12(OH)12 exists, and its characterization leaves much to question. In a 4-month reaction, we synthesized this reported compound and found that the highly crystalline material was black with a very broad solid-state absorbance from 300 to 1300 nm, unlike any other known molecular dodecaborate radical. We further explore the magnetic, electronic, and crystallographic properties of this compound and find that the radical compound is impure even in the single crystalline state.
Victor de Sousa	**Influence of Ligand Cross-Link Length on Secondary Building Unit Formation in OligoMOFs**	OligoMOFs are a new category of Metal-Organic Frameworks (MOFs) that feature ligands covalently cross-linked into oligomers as intrinsic structural components. Recent studies have demonstrated that the size and flexibility of tether moieties can result in the formation of OligoMOFs with different isomeric structures by causing distortions in the secondary building unit (SBU).1 In this work, we demonstrate that using tethered dimeric ligands with subtly different carbon chain lengths can yield OligoMOFs with chemically distinct secondary building units (SBUs) and distinct structures. Specifically, we find that terephthalate dimers with hexyl and heptyl spacers form oligoMOFs [Zn_2(hexyl(bdc)2)$(bpy)_2$] and [Zn_2(heptyl(bdc)2)$(bpy)_2$] when combined with Zn2+ and 4,4'-bipyridine (bpy). Notably, the hexyl tether results in a framework structure identical to MOF-508a, based on dinuclear {Zn2} "paddlewheel" SBUs,2 while the heptyl tether results in a "honeycomb-like" framework structure based on an infinite rod-like Zn2+ SBU bridged by ligand carboxylate groups.3 These results represent the first examples of tether length influencing SBU chemistry in MOFs and constitute a step forward in understanding the interplay between the MOF lattice and the geometric constraints imposed by inter-ligand cross-links. 1. Sensharma and Cohen, Chem. Sci., 2024,15, 20448-20456. 2. Chen, Yaghi, et al., Angew. Chem. Int. Ed., 2006, 45, 1390-1393. 3. Henke and Fischer, J. Am. Chem. Soc. 2011, 133, 7, 2064–2067

Vivek Vasudev	**A new class of photochromes for ultrastable switching and photomechanical motion**	Molecular photoswitches are photochromic organic compounds that undergo reversible photoisomerization, enabling them to alter their molecular properties. Although azobenzene derivatives have been extensively explored, high thermal stability and shifting absorption into the far-red region remain challenging. Herein, we introduce a family of divinyl derivatives with asymmetric substitution, designed to enhance absorption in the visible region. These derivatives consist of a light-absorbing PAH sail and an isomerizing tail, with tunable absorption properties that vary based on the PAH unit. Notably, the cis form remains stable even at elevated temperatures of up to 90°C. The detailed analysis demonstrates photoisomerization in both directions (E→Z and Z→E), with the quantum yields ranging from 0.1 to 0.5. Time-resolved spectroscopy measurements indicate that the photoisomerization reactions take place within the range of 10-20 ps. This innovative class of light-activated switches is a valuable expansion to the limited repository of bistable photochromic compounds.
Vivian Yuen	**Synthesis and Characterization of Trimetallic Complexes containing Triptycene-based Redox-Active Ligands**	Triptycene-based ligands are commonly used as redox-active organic linkers in 2D metal-organic frameworks (MOFs) due to their electronic tunability. To date, there are no fundamental studies examining the influence of tuning the coordination environment of molecular complexes with triptycene-based redox-active ligands on the bulk properties of assembled MOFs. Using a bottom-up synthetic approach, I aim to investigate the electronic and structural properties of molecular analogues to triptycene-based bulk materials in hopes of constructing synthetically tunable MOFs. In this talk, I discuss the synthesis and characterization of trimetallic complexes containing triptycene tris-catecholate redox-active ligands and efforts to elucidate the electronic properties of these molecular analogues to 2D-MOFs.

William Ragen	**Optical & chemical transformations from day- and night-aged nitrate-oxidized pyrrole brown carbon aerosols**	Pyrrole is a heterocyclic volatile organic compound (VOC) emitted into the atmosphere through processes like biomass burning and microbial decomposition. Pyrrole can readily react with atmospheric nitrate radicals (NO3) during nighttime to form secondary brown carbon (BrC) aerosols. The evolution of BrC from the NO3 oxidation of heterocyclic VOCs during chemical aging has not been extensively studied. In this work, we carried out experiments in a 10 m^3 smog chamber to investigate the evolution of chemical composition and optical properties resulting from NO3- and OH-induced aging of BrC from the NO3 oxidation of pyrrole. The chemical composition and optical properties of the aged BrC were characterized using a suite of online and offline instrumentation. Our results show that compared to the SOA from initial NO3 oxidation, the bulk mass absorption coefficient (<MACbulk>) of aged SOA shows an 8% decrease from OH aging and a 21% decrease from NO3 aging on average. Several monomeric and dimeric products, likely light-absorbing species, were measured by mass spectrometry. Analysis of gas- and particle-phase chemical composition before and after aging suggests that strongly absorbing chromophores are consumed to produce less absorbing dimer products, likely phthalimides. This dimerization process is suggested to occur to a larger extent in the NO3-induced aging, responsible for the larger decrease in light absorption. Overall, this study expands the understanding of chromophores from the NO3 oxidation of pyrroles and helps elucidate how these chromophores evolve during daytime and nighttime aging.
Ye Wen	**Understanding Hardness Mechanisms in Metal Dodecaborides Using Machine Learning Modeling and Simulations**	Transition metal borides are superhard materials (Vickers Hardness ≥ 40GPa) that offer ambient synthesis alternatives to traditional abrasive materials like diamond and cBN. Of these materials, zirconium dodecaboride solid solutions have promising cost-to-hardness ratios. Past work by the Tolbert group has identified a compactness (deviation from ideal volume) in these materials. While a positive correlation between compactness and hardness has been established, there lacks a connection between composition and compactness. We aim to bridge the missing connection using machine learning (ML) approaches on a dataset of 54 experimentally-derived datapoints. We proposed a new metric to calculate the volume deviation (ΔV), which improves compatibility with regression models, yielding an R2 = 0.51 compared to the original R2 = 0.20 from models trained on compactness. ΔV remains a good indication of compactness as it forms a strong quadratic relationship when plotted against compactness. A tuned quadratic model was implemented, which further improved R2 = 0.66 and provided insights into the compactness contributions of binary elemental combinations. We expect the implementation of an “activity coefficient” to further improve the fit. Lastly, to determine the root mechanism and improve model training data, we implemented an ML-based atomic potential calculator, MACE, to reproduce experimental results. Monte Carlo and strain simulations were performed to investigate the energetic effects of both disordered and ordered materials.

Yin Pok Wong	**Catalyst repurposing with network science across dissimilar reaction domains**	In this work, we have established the fundamental principles of a catalyst-reaction network by framing the relationship between ligands and reactions with a bipartite network and used modern link prediction techniques to create a powerful recommender for users to repurpose previously synthesized catalysts for untested reactions. With this workflow, we identified repurposed catalyst designs for nickel catalyzed CO2 and ethylene coupling to form acrylate, as well as CO and ethylene copolymerization for polyketone synthesis. We envision that this methodology can be used to accelerate catalyst discovery, particularly when the number of known catalysts is scarce. In addition, we believe that catalyst repurposing would bring a new paradigm for catalyst discovery, as it would be faster than traditional process of catalyst development based on novel catalyst development.
Zoe Heidersbach	**Co-Oligomerization of Alpha- and Beta-Synuclein with Epigallocatechin Gallate**	Alpha-synuclein (α-syn), an intrinsically disordered protein, plays a critical role in Parkinson's Disease by aggregating into amyloid fibrils that disrupt cellular membranes and accumulate in the brain. The green tea–derived small molecule epigallocatechin gallate (EGCG) inhibits α-syn aggregation in vitro. Beta-synuclein (β-syn), a closely related paralog, does not form pathogenic fibrils and may interfere with α-syn aggregation, potentially by forming off-pathway small oligomers. If true, co-incubation of α-syn with β-syn should yield mixed oligomers containing both proteins. Native and denatured electrospray ionization mass spectrometry (ESI-MS) was used to characterize monomeric and small oligomeric species formed from co-incubation of α-syn and β-syn, as well as their interactions with EGCG. Results showed that α-syn binds one EGCG molecule covalently, with additional nonspecific binding of a second EGCG possible. In contrast, β-syn binds up to four EGCG molecules, with two involving covalent interactions. By 24 hours of incubation, heterodimers of α-syn and β-syn were detectable, suggesting hetero-oligomerization as a possible mechanism of aggregation inhibition. Gamma-synuclein (γ-syn), another paralog sharing a key 11-residue segment (residues 74–84 in the NAC region) with α-syn—but not β-syn—did not form heterodimers with α-syn during this time frame. This implies that the NAC segment is critical for the inhibitory interaction between α-syn and β-syn. Current work is extending this analysis to 72–120-hour incubations to track the development of larger oligomers, the potential for hetero-oligomer formation, and EGCG's ability to bind these higher-order species.

Zulfiqar Mohamedshah	**Highly Efficient Expression of DNA-peptide Conjugates in Growth-arrested Cells**	Efficient nuclear delivery of DNA remains a major challenge in non-viral gene therapy. While nuclear localization signal (NLS) peptides have been explored for enhancing nuclear translocation of DNA, their efficacy has been limited by DNA-peptide conjugation strategies. Leveraging E. coli tRNA guanine transglycosylase (TGT), we present a modular workflow for generating DNA oligonucleotide-peptide conjugates which are ligated to linear DNA to generate peptide-modified gene cassettes (DNA-PepTAG). Using an eGFP reporter system, we optimized the linker length between DNA and the NLS peptide and determined that a single NLS modification significantly enhances expression up to ~10-fold, whereas dual modifications on opposite ends drastically reduce it. Screening multiple NLS peptides in growth-arrested human cell lines revealed cell-type-specific preferences for nuclear translocation of DNA cargo. Two NLS peptides, PLSCR-1 and extSV40, exhibited consistently high expression across tested cell types, indicating broad applicability for nuclear delivery. We evaluated the generality of our approach by delivering both cytosolic and secreted DNA payloads, as well as gene cassettes that range in size from 1.3 kbp to 7 kbp. Furthermore, in a direct comparison with previous strategies, our method of generating NLS tagged gene cassettes proved to be consistently superior. These findings support the potential of DNA-NLS conjugates generated via DNA-PepTAG as a viable strategy for non-viral gene therapy, enabling enhanced nuclear delivery of therapeutic genes while minimizing the required DNA dose.