University of Rochester
Chemistry Newsletter 2019-2023

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From the Chair

Greetings Chemistry Department alumni, faculty, students and staff! We are very happy to publish our Newsletter again after a hiatus. I have heard how much our Newsletter is anticipated and appreciated by alumni and friends of the Department, which makes me even more excited to get back in touch with developments in UR Chemistry. Herein, we report Department highlights since 2019, but focus on 2022 – 2023.

First, I want to thank Todd Krauss, who preceded me as Department Chair from 2013-2022. Todd led our department for three terms with great energy and enthusiasm. He oversaw the successful hiring of six of our current tenure-track faculty at the Assistant Professor level, despite the challenging environment presented by the Covid-19 pandemic. We are grateful to Todd for his outstanding leadership during those difficult times. In addition to faculty hiring, Todd was highly successful in fundraising, with three new endowed chemistry Chairs coming online: the Boeckman, the Eisenberg, and the Marvin Chairs. These Chairs provide support that will further advance our efforts to build a talented faculty, and I comment further on these below.

With a heavy heart, we mark the passing of two of our faculty emeriti. In June 2019, Professor Emeritus William Saunders passed away. Prof. Saunders was hired by Albert Noyes to join the Department in 1953 and established an impactful research program in which he interrogated reaction mechanisms with great rigor. He also served as Department Chair from 1966 to 1970. In 1991, he entered the Senior Faculty Associates Program and remained active in the Department. We greatly miss his enthusiastic participation in Department activities.

In September, 2021, we sadly lost Robert K. Boeckman, Jr., Marshall D. Gates Professor of Chemistry Emeritus. Bob joined the Department in 1980 and quickly built a large and high-profile research group that made major contributions to the area of synthetic organic chemistry. His work was recognized by many prestigious awards, and he also served as an Associate Editor for the *Journal of Organic Chemistry*. One of Bob's major impacts was his service to the Department as Chair from 2003 to 2013, during which he worked to establish the Kende and Eisenberg endowed Chairs. The generosity of Bob and his spouse Mary Delton led to the establishment of the Robert K. Boeckman, Jr. and Mary H. Delton Family Distinguished Professorship in Organic Chemistry.

The Department has welcomed seven new tenure-track faculty since 2019; five at the junior level and two at the senior level, as well as a new teaching faculty member. Starting with the tenure-track Assistant Professor hires, in 2020, UR alumna C. Rose Kennedy joined us and is growing a research program focused on developing sustainable catalytic methods that spans organic and inorganic chemistry. In 2021, we welcomed Brandon Barnett, whose work bridges organometallic and inorganic materials chemistry to investigate oxidation catalysis and to perform challenging molecular separations. Further expanding our footprint in materials chemistry, Benjamin Partridge joined our faculty in 2022, bringing his experience in supramolecular chemistry to develop dynamic assemblies inspired by nature. In 2023, we welcomed Agnes Thorarinsdottir, who is designing new electrochemical systems to address problems in energy and sustainability. And in 2024 we will welcome Yishu Jiang, who is setting up her biophysical chemistry lab centered on studying, using, and creating excited states in biological systems. We are thrilled to have identified all of this outstanding talent! We have also brought on board one senior teaching-track hire and two senior tenure-track hires. Bringing significant experience in education, Megan Tichy has joined us as of August 2024 as a Professor of Instruction, moving to Rochester from Santa Clara University. We also hired two faculty with tenure. Michael Ruggiero moved from the University of Vermont in 2023, bringing his expertise in terahertz spectroscopy, a method well suited for studying materials. We also were thrilled to welcome Professor. Nicole Sampson, who was hired to be the Robert L. and Mary L. Sproull Dean of the School of Arts and Sciences, and also a Professor of Chemistry. Prof. Sampson also is continuing her NIH-funded research on the use of polymers to activate and inhibit receptors that play a range of biological roles. Recently, it was announced that Dean Sampson will serve as Interim Provost, and we congratulate her on her new role!

These hires have transformed our Department. One effect is significant growth in the area of materials chemistry, with strengths in synthesis and application of both "hard" and "soft" materials, as well as development of methods for characterizing these complex systems. These hires also further strengthen our Department's

efforts in the area of catalysis, with applications in human health and in sustainability. Furthermore, this influx of early-career faculty gives our Department palpable energy! Finally, we are thrilled to note that we are approaching gender parity in our tenure-track faculty, now with 9 women out of 21 faculty, making us one of the top Chemistry Departments where it comes to representation of women on the faculty.

Turning now to retirements and departures, we celebrate the career of Doug Turner, our faculty member who entered emeritus status since publication of the 2018 Newsletter. Doug is internationally known for his groundbreaking contributions to understanding the thermodynamics of RNA folding, work that formed a foundation for the development of mRNA vaccines against Covid-19. The faculty also bid farewell to Rudi Fasan and Michael Neidig who departed for the University of Texas, Dallas, and Oxford, respectively. We expect to see the programs that they established at UR continue to thrive in their new homes.

Our Department would grind to a halt if not for the work of our outstanding staff. We were happy to welcome Elaine Maholick (Undergraduate Coordinator), Emily Breitbart (Graduate Coordinator), and Jason Holt (Senior Laboratory Engineer). We have also had several staff retirements. Long-time technical staff members Eric Lobenstine and Pete Serrino entered retirement, as did Linda Boyle and Anna Kuitems from the Business Office. We are deeply grateful for their decades of service that supported our students and faculty in myriad ways. I also wish to recognize the passing of Debra Haring in 2022, who was our fantastic Development Administrator from 2005-2010, after which she moved to the Dean's office. We continued to work with Debra in her new position as she led many major grant writing efforts. She is deeply missed.

As noted above, we have grown our endowed professorships in our Department thanks to the donations of alumni, faculty, and other friends of the Department. A generous gift from Dr. Dean Marvin '73 and Mrs. Laura Marvin endowed the Marvin Professorship in Physical Chemistry. Currently, these funds are supporting Professor Jiang, who has been named a Marvin Fellow. We look forward to filling this professorship in the future. The gift from the Marvins also has supported summer undergraduate research. Their generosity has positively impacted groups across the Department and helped us build in physical chemistry! The Richard S. Eisenberg Professorship in Chemistry also was established, thanks to the generosity of Rich and Marcia Eisenberg as well as many colleagues and alumni. I was incredibly honored to be named the inaugural Eisenberg Professor in 2021.

The research of many of our faculty was recognized through promotions (Knowles, Franco, Huo, Matson, Nilsson), named professorships (Matson as the Marshall D. Gates, Jr. Professor in Chemistry and Krauss as the Jay Last Professor in Arts, Sciences & Engineering), grants, and awards. Given the scope of this update, I can't name all of these here and refer you to our updates throughout this Newsletter, though I will mention a few highlights. One is that Professor Rose Kennedy was named one of 20 Packard Fellows Nationwide in 2022, a great achievement. Another major accomplishment is the election of Professor Bill Jones to the National Academy of Sciences, one of the highest honors a scientist can earn. We are incredibly proud of the achievements of all of our Department members!

Finally, I want to thank all who have supported our Department. One of the unexpected pleasant surprises that has come from being Chair was a big increase in interactions with friends and alumni of our Department. We appreciate your feedback and support. Our "Chemistry Alumni Research Fund" is a great resource for the Department as it enables us to pursue a number of impactful endeavors, most notably student fellowship awards, research, education, and travel. Unlike the "Dean's Fund for Chemistry," which is not under the purview of the Department, "Chemistry Alumni Research Fund" gives us additional resources we can leverage to the advantage of the faculty and students in the Department, and we appreciate your support of this fund.

Best wishes and we hope to see you at an upcoming Meliora Weekend!

Kara L. Bren

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Your Cause

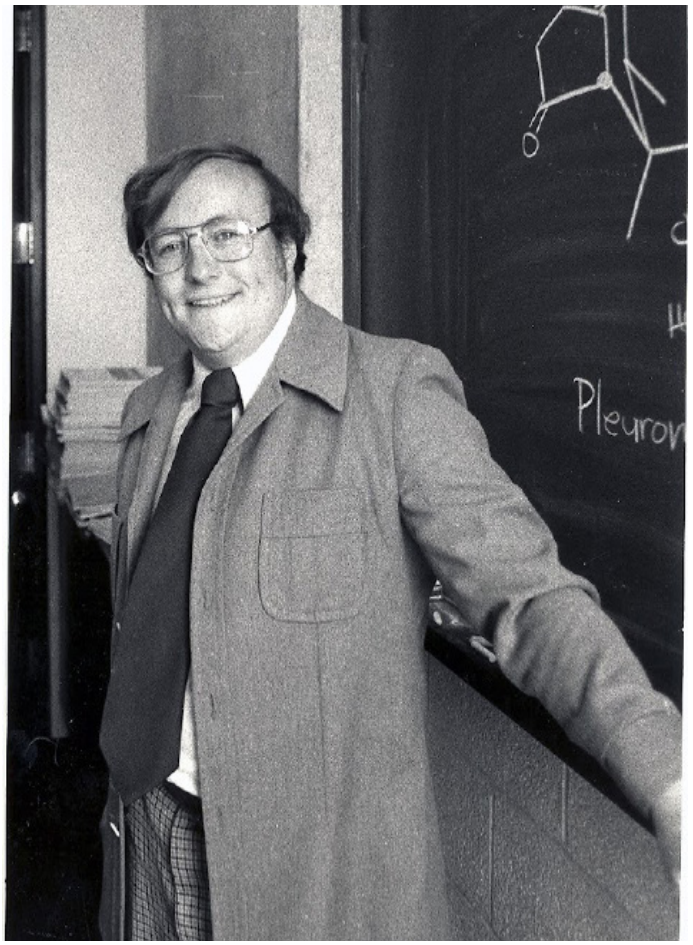
In Memoriam
Robert K. Boeckman, Jr.

It is with deep sorrow that we mourn the passing of Professor Emeritus Robert K. Boeckman, Jr. on September 5, 2021. Bob is survived by his wife of over 45 years, Mary Delton. Bob met Mary at a chemistry conference in Kingston, Jamaica in January 1976. They were married the following June. They shared a love of science, horses, cats, and nature. They moved to the Adirondacks upon Bob's retirement in July 2019.

Bob was born on August 26, 1944, in Pasadena, California while his father was stationed there during WWII. After early schooling in Dayton, Ohio, Bob received his bachelor of science in chemistry in 1966 from Carnegie Institute of Technology (now Carnegie Mellon University). He moved on to Brandeis University where he received his Ph.D. under the supervision of James B. Hendrickson and Ernest Grunwald in 1970. Bob went on to complete his postdoctoral studies with Gilbert Stork at Columbia University. He began his academic career at Wayne State University in 1972, where he rose to the rank of Professor in 1979. In 1980, he joined the faculty of the University of Rochester.

For decades, Bob operated one of the largest research groups in the Chemistry Department and coauthored over 150 research papers and book chapters with his students and postdoctoral associates, principally in the area of synthetic organic chemistry. His impressive research accomplishments included specializing in the first total syntheses of well over a dozen major complex natural product targets, and completing about three dozen total syntheses of such targets.

In 2003, Bob became the inaugural holder of the Marshall D. Gates Endowed Chair, a fantastic honor in light of Marshall's lifetime commitment to the area of total synthesis. Bob's other academic honors included an A.P. Sloan Fellowship, a Research Career Development Award from the National Institutes of Health, and an ACS Cope Scholar Award. He was a fellow of the Japanese Society for the Promotion of Science, was twice awarded an Alexander Von Humboldt Stiftung Research Prize for Senior Scientists, and was an inaugural ACS fellow and a fellow of the AAAS. From 1997 until 2016, he served as an associate editor of the *Journal of Organic Chemistry*. Bob's scientific achievements were coupled with a strong commitment to graduate teaching and mentorship. This culminated in Bob winning the William H. Riker University Award for Graduate Teaching in 2009.



Bob also gave much of his time in service, especially to the Chemistry Department and the greater University. From 2003 to 2013, Bob was the Chair of the Department. Among his more notable accomplishments during this time was the establishment of the biological and materials interdisciplinary clusters, whereby for the first time, faculty outside the core chemistry faculty were integrated into the activities of the Chemistry Department. Some of Bob's most impactful efforts as Chair were achieved through his unique success in raising endowed funds for the Chemistry Department. In particular, by working with the University's advancement office, Bob was integral in the establishment of two endowed professorships: the Andrew Kende Chair of Organic Chemistry honoring our late colleague, and the Richard S. Eisenberg Professorship of Chemistry. Bob has bequeathed an endowed Professorship to the Chemistry Department of the University of Rochester in his name.

In addition to Bob's chemistry endeavors, he was a long-term supporter and President of Pet Pride of New York, Inc., a no-kill, cats only, sanctuary and adoption center. During his tenure, the organization blossomed, adopting over 200 cats and kittens in 2020.

On Friday June 14, 2019, a retirement celebration was held for Bob at Oak Hill Country Club. As part of this celebration the department hosted a symposium with invited speakers, his former students, and colleagues to honor Bob's extraordinary contributions to the University of Rochester. Bob retired from the University in July 2019 with Emeritus status as the Marshall D. Gates, Jr. Professor of Chemistry. He remained active in his discipline, still working on a medicinal chemistry research project of bisphosphonates and bisphosphonate drug conjugates at the time of his death.

Bob is missed by not only his friends and family and colleagues, but also the greater chemistry community worldwide.

In Memoriam William Saunders

The Chemistry Department continues to mourn the loss of Emeritus Professor William "Bill" H. Saunders, Jr. who passed away in Rochester, NY on Monday, June 17, 2019, at the age of 93.

Bill was born in Pulaski, Virginia and graduated from the College of William and Mary with a degree in chemistry after serving two years in the U.S. Army from 1944 to 1946. When he returned to the U.S., Bill went on to graduate studies in chemistry at Northwestern University followed by a move to MIT for postdoctoral work. After completing his postdoctoral studies, Bill was hired by Albert Noyes and joined the University of Rochester Chemistry Department in 1953. Bill served as department chair from 1966 to 1970 and recruited Tom Krugh, Andy Kende, and Keiji Morokuma to the Department.

Bill's first paper from Rochester used sulfur isotope effects to probe the transition state structure in the elimination of b-phenethyl sulfonium salts. This work exemplifies two continuing themes that occupied Bill for much of his career in chemistry: kinetic isotope effects and elimination reactions.

In 1991, Bill transitioned to the status of Senior Faculty Associate, which meant practically that he retired from teaching and experimental research. However, Bill began a new career as an expert computational chemist interested in valence bond calculations. Bill published his first paper in 1953 and his latest contribution to the literature was in 2015 -- a remarkable time span of 62 years!

Bill married Nina Plesums in 1960 and raised two children, Anne and Claude, inculcating in them a love for learning and the arts. After Nina died in 1982, he remained single for 20 years but kept busy not only with research and teaching, but also international bike trips, cross-country skiing, visits to the Finger Lakes wineries, and frequent concerts and theater performances. He met his second wife, Barbara, through friends at First Unitarian Church in Rochester. They married in 2002 and shared their love of travel, visiting many places in the U.S. and abroad. Cancer struck as they were planning a trip to China in 2004, and Barbara died in 2005.

The Chemistry department faculty and some special guests gathered together on Thursday, August 1, 2016 at the Next Door Bar and Grill in Pittsford to celebrate Bill's 90th birthday. Joining the faculty were Bill's two children, Anne and Claude, and former doctoral students Dr. Fred Lewis (Ph.D. '68) and Dr. Karen Hill Brown (Ph.D. '72). Professor Joe Dinnocenzo emceed the event and introduced Fred and Karen, who told some great stories from their graduate school days. Anne and Claude Saunders also shared some stories from their childhood and what it was like having Bill as a father. It seems that he was a big Monty Python fan and passed it on to his children.

Professor Saunders is sitting in the middle of the couch on the right.

In Memoriam Debra Haring

Debra Fran Haring passed away on December 27, 2022, at the age of 65 after a courageous battle with brain cancer. Throughout her illness, Debra remained hopeful and positive despite the health challenges that she was facing. She was truly an inspiration to those who were fortunate to know her and love her.

Debra worked in the Chemistry Department for ten years, first as administrative assistant to Professor Shaul Mukamel and later as development administrator. Debra bid a very fond farewell to the Chemistry Department on February 1, 2010 to pursue a new position in the School of Arts, Sciences, and Engineering as the Assistant Dean of Grants and Contracts. Debra developed this new position which provides extensive pre-proposal grant support to faculty and staff across a broad range of departments and programs representing all the Humanities, Social Science and Science disciplines at UR. She also served as an additional resource for faculty and administrative staff for pre- and post-award compliance, and as a liaison with the Office of Research and Project Administration and Foundation and Corporate Relations at the University. The expertise and 'best practices' that Debra gained during her years in the Chemistry Department informed her new role at the College, and she remained in close contact by assisting with multi-departmental grants involving Chemistry faculty. In addition to the exciting promotion to the Deans' Office, Debra was honored in 2009 with the Witmer Award for Distinguished Service. Debra was also instrumental in the Arts, Sciences and Engineering's Research Office Team, receiving the 2017 Meliora Team Award.

In October 2023, the Debra Haring Excellence in Research Award was created to honor Debra's legacy which is evident everyday in the research accomplishments of the faculty and their success at obtaining funding, and also in the interdisciplinary connections that have been made among faculty. This award will ensure that Debra's legacy, her strong work ethic, intelligence, humor and kindness live on for generations to come. The award will recognize a faculty member who has done research that has had a transformational impact or has changed their field in positive ways.

Debra is survived by her husband, Cornelis "Cook" Haring and their four children, four grandchildren, two sisters, one brother and many nieces, nephews and dear friends. Debra's greatest love was her family. She was a devoted wife, mother, grandmother, aunt, sister and daughter. Debra's Jewish identity and strong spiritual connection with Israel shaped her values and the way she led her life. Debra and her extended family enjoyed making lifelong memories at their family's Owasco lake house. Debra was a beloved friend and colleague who formed lifelong bonds with those who were closest to her and her memory will live on in their hearts and minds.

Debra Haring

Faculty News

Brandon Barnett

Assistant Professor of Chemistry

Ph.D. 2016, University of California, San Diego

RESEARCH INTERESTS

Interested in coordination chemistry relevant to oxidation catalysis, as well as adsorbent technology for the point-source capture of greenhouse gases. Work lies at the interface of organometallic and inorganic materials chemistry.

CONTACT

brandon.barnett@rochester.edu

The past year was full of important landmarks for the **BARNETT** group. After a COVID-caused delay, the group moved into its newly renovated laboratory and office spaces (Hutchison B02, B19, B20), modules that formerly housed the Farrar group. Moving into its "forever home" allowed the group to install and christen the remainder of its instrumentation and reach full research capacity.

Earlier this year, the group published its inaugural paper in *Inorganic Chemistry* (Brandon was thrilled to see Paper #1 end up in the journal that was led by Rich Eisenberg as EIC for over a decade!). This work, funded by both the University and a grant from the ACS Petroleum Research Fund, represented an important achievement in ligand design – one that will underpin a significant portion of the group's work for years to come. Work on this project has been led by graduate student **CHRIS HASTINGS** (a 2022 Weissberger Fellow!) and graduate student **LUCY HUFFMAN** (a 2023 Sherman-Clarke Fellow!), with additional contributions from undergraduates **PAUL YOON** ('24) and **MARINA ZAPESOCHNY** ('25).

Additional ongoing work involves the use of porous sorbent materials for the capture of "super greenhouse gases" from point emission sources. Although emitted in far smaller quantities than CO_2, small fluorinated gases with important industrial uses have outsized contributions to the atmosphere's heat-trapping capacity. The group seeks to develop materials capable of capturing these fluorinated gases prior to their venting into the atmosphere, decreasing the carbon footprint of important industrial sectors (e.g. semiconductor fabrication) and potentially allowing for the recycling and reuse of these expensive gases. The group is about to submit its first paper on this topic for publication. Work has been led by graduate student **BEVAN WHITEHEAD** (a 2023 DeRight Fellow!), with additional contributions from undergraduates **HOPE SILVA** ('24) and **MIRANDA STEWART** ('25).

In addition to the above student fellowship successes, several other group members have received exciting recognitions. Hope Silva was awarded a prestigious Goldwater Scholarship as part of an impressive cohort of UofR nominees that went 4/4 in the national competition. Hope additionally won travel awards from both the UofR Office of Undergraduate Research and the ACS Division of Inorganic Chemistry, which funded her recent trip to the ACS National Meeting in San Francisco to present her latest results. Finally, three group members (Hope Silva, Miranda Stewart, and Marina Zapesochny) were awarded the Schwartz Discover Grant, which helped to fund their research in the lab over the summer.

Brandon has enjoyed beginning to travel and show off the group's work. Over the last 15 months, he has spoken in the "Emerging Areas in Inorganic Chemistry" symposium at the Chicago ACS National Meeting, and has given presentations at the Organometallics Gordon Research Conference and the San Francisco ACS National Meeting. He is excited to see what the next year brings for the group!

L to R: Hope Silva (BS '24), Chris Hastings, Lucy Huffman, Brandon Barnett, Miranda Stewart ('25), Marina Zapesochny ('25), Bevan Whitehead, Bob (dog)

Kara L. Bren

Professor of Chemistry

Ph.D. 1996, California Institute of Technology

RESEARCH INTERESTS

Interested in bioinorganic/biophysical chemistry. Emphasizes the development of artificial enzymes that catalyze the reduction of protons derived from water to hydrogen. The goal is to produce elegant and efficient systems that perform artificial photosynthesis.

CONTACT

kara.bren@rochester.edu

The **BREN** Group has been expanding its research activities in multiple areas. An overall goal of the group's work is to develop novel bioinspired and biological systems for converting low-energy, inexpensive substrates into valuable products. While the group has a long-standing program in developing and studying catalysts for hydrogen (H_2) production from water, they have also been developing new (to them) transformations, particularly converting nitrogen oxyanion pollutants such as nitrite and nitrate into the valuable products hydroxylamine and ammonia and reducing carbon dioxide into the fuel precursor carbon monoxide. An exciting new development is that the group's work on developing living bio-nano systems for photocatalytic hydrogen production from water received support from the Department of Energy in a project led by Kara along with co-investigators Todd Krauss, Anne Meyer (Biology) and Andrew White (Chemical Engineering).

Bren group students have been busy keeping these projects moving forward. Senior PhD student **JI WON HAN** has been leading efforts in studying metallopeptide and metalloprotein catalysts for electrochemical and photochemical proton and carbon dioxide reduction. One of her major contributions was demonstrating how metallopeptide structure impacts catalytic activity toward proton reduction. Ji won also has been a fantastic teacher and mentor in the group and has laid the foundation for the next generation of systems for study. Another senior PhD student in the lab and NSF Graduate Fellow, **ALISON SALAMATIAN**, has been the lab's pioneer and specialist in developing systems for carbon dioxide reduction. Alison's work has shown that engineered biocatalysts can perform selective carbon dioxide reduction in water, conditions in which competition from proton reduction represents a major challenge. PhD student **KAYE KUPHAL** has been the group's leader in nitrogen oxyanion reduction and has developed a system using an iron catalyst for converting the pollutant nitrate into energy-rich, useful products. Kaye has creatively demonstrated use of her iron catalyst for other reactions relevant to the nitrogen cycle and carbon-free fuel use. **RYAN KOSKO**, also a fourth-year PhD student, has been pushing forward aspects of two projects in photocatalysis: developing living bio-nano systems for hydrogen production, and investigating the mechanism of photocatalytic hydrogen production in organic dye-protein complexes. Ryan was awarded a prestigious Hooker Fellowship for his work. Also joining the living bio-nano solar fuel project is PhD student **SORAYA NGARNIM**, who is the group's specialist in investigating properties of these systems using a combination of photochemistry, spectroscopy, microscopy, and electrochemistry. Soraya has shown great resourcefulness in this challenging work. PhD student **HAFSA IRFAN** has been developing new metallopeptide and protein catalysts and investigating factors controlling activity of quantum-dot-based systems for photochemical hydrogen production in collaboration with the Krauss lab. Hafsa has also engineered highly active and selective new protein catalysts for carbon dioxide reduction. **MARIA FERNANDA (MAFE) LIZARAZO**, also a PhD student, has contributed to two directions in carbon-free fuel production: investigating nitrate reduction in collaboration with Kaye and pairing engineered biocatalysts with quantum dots to yield new hybrid photocatalytic systems. The group has also been fortunate to have undergraduate **HAFSA MOHAMED** working with us. Hafsa has worked closely with Alison on carbon dioxide reduction, providing exciting results on photochemical systems.

The Bren group also celebrated exciting news from alumni in recent years. They were thrilled to hear that **BANU KANDEMIR QEMO** (PhD '16, Postdoc '20, and Senior Scientist at QuidelOrtho), welcomed her daughter Leila into the world! We also celebrated new positions and promotions for alumni: **AMY ENSIGN KOVACH** (PhD '09) took on a new challenge as Vice President of Academic Affairs at Mount Vernon Nazarene University in Ohio, and **LEA VACCA MICHEL** (PhD '07) and **MATTHEW LIPTAK** (Postdoc '11) were promoted to Full Professor at RIT and the University of Vermont, respectively. More recent graduates have also been getting their careers off to a great start. **EMILY EDWARDS** (PhD '22) took a position as Scientific Editor for *Cell Reports Physical Science* and **JESSE STROKA** (PhD '21) is a Scientist at Bausch and Lomb.

Kara's biggest new change has been taking on the role of Department Chair, which she stepped into in January 2022. She has particularly enjoyed getting to know staff better and working to hire outstanding faculty into the department. Kara has also continued in her role of Associate Editor for the *Journal of the American Chemical Society* and has enjoyed attending conferences again, with highlights including the Latin American Meeting on Biological Inorganic Chemistry in Viña del Mar, Chile; a Telluride Workshop on Proton-Coupled Electron Transfer, and Bioinorganic Symposia in Jeonju and Gwangju, Korea. Early 2024 saw her traveling to India for the Symposium for Advanced Bioinorganic Chemistry and speaking at the Renewable Energy Gordon Research Conference.

Kara's most exciting happening in 2023 was being inducted into the American Academy of Arts and Sciences, in a Fall ceremony in Cambridge, MA, which was attended by her husband Jim Java and colleagues and friends Bill and Heather Jones. She's excited to become part of this stimulating and diverse society which has already helped her make connections with scholars in a wide range of disciplines.

Back row L to R: Kara Bren, Ryan Kosko, Jiwon Han, Soraya Ngarnim
Front row L to R: Cooper, Kaye Kuphal, Alison Salamatian, Hafsa Irfan, Mafe Lizarazo

Joseph P. Dinnocenzo

Professor of Chemistry

Ph.D. 1983, Cornell University

RESEARCH INTERESTS

Chemistry of organic ion radicals; mechanistic and physical organic chemistry; design and testing of new photoresponsive polymeric materials.

CONTACT

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JOE DINNOCENZO and his group are continuing research on organic exciplexes with novel charge types (cationic, anionic, and neutral). Joe enjoys working in the lab on a regular basis and has been fortunate to continue his collaboration with Samir Farid on the exciplex project, work that is funded by a grant from the National Science Foundation (NSF).

In a second project funded by the NSF, Joe has been collaborating with Dr. Cecilia Barone and her colleagues in UofR's Learning Center on a project to develop a new video-based training resource for Peer-Led Team Learning (PLTL) that helps PLTL leaders recognize visible and invisible barriers to participation experienced by students in diverse STEM teams. In late May, the University will host the Peer-Led Team Learning International Society conference where they will hold a workshop to train PLTL practioners from around the world to use this new resource.

Joe has been teaching the large sophomore organic chemistry course for the past two years. The experience is both exhilarating and exhausting! Joe looks forward to teaching the course again this fall and to working with another group of stimulating PLTL leaders and students.


THIS HALL, BUILT 1968-71,
IS NAMED IN HONOR OF
CHARLES FORCE HUTCHISON
TRUSTEE OF THE UNIVERSITY SINCE 1932
BORN IN ROCHESTER IN 1875
STUDENT AT THE UNIVERSITY 1895-99
PIONEER IN PHOTOGRAPHY
WISE IN COUNSEL, BOLD IN VISION,
STEADFAST IN ADVERSITY,
UNSURPASSED IN LOYALTY
AND LOVE TO HIS UNIVERSITY
DEDICATED OCTOBER, 1971

Ignacio Franco

Associate Professor of Chemistry — Ph.D. 2007, University of Toronto

RESEARCH INTERESTS

Laser control of electronic properties and dynamics, electronic decoherence in molecules, theory and simulation of single-molecule pulling processes, novel spectroscopies and control in single-molecule junctions.

CONTACT

ignacio.franco@rochester.edu

The **FRANCO** group is a theoretical physical chemistry group working in the general area of quantum dynamics and molecular modeling. The work of our group encompasses the development of new theories and simulation methods, the efficient implementation of these methods on high-performance computers, and the application of the resulting tools to identify new phenomenology, and understand and stimulate experiments. We work closely with experimental groups and strive to perform theory that stimulates experimental progress. This summer the group turned 10 years old! It's been ten very exciting years pushing quantum frontiers in molecular and material science.

Here are some exciting recent discoveries by the Franco group. In a paper recently published in *Nature*, **ANTONIO GARZON-RAMIREZ** developed the theory behind laser experiments demonstrating information processing at femtosecond (a millionth of a billionth of a second) time scales! This development is the foundation of future electronics and computation operating at the petahertz limit, six orders of magnitude faster than the state-of-the-art. In a paper in *Nature Communications*, **LEOPOLDO MEJIA** developed the microscopic theory of conductance lineshapes in molecular electronics experiments by combining molecular conductance with the theory of force spectroscopy. This development augments the information that can be extracted from this class of experiments and may lead to conductance spectroscopies of enhanced resolution. In a recent *J. Phys. Chem. Lett.,* **WENXIAN HU** showed how to enhance the quantum coherence of matter by orders of magnitude (!) by hybridizing molecular states with those of quantum light. In a recent *PRX Quantum* (editor's choice), **CHANG WOO KIM** demonstrated how to create an analog quantum simulator for open quantum systems by mapping chemical dynamics to a highly controllable quantum hardware. Writing in *Phys. Rev. B*, **VISHAL TIWARI** showed how to create novel non-equilibrium materials with effective properties that can be triggered on demand by dressing them with light. **IGNACIO GUSTIN** demonstrated how to identify how quantum coherence is lost in molecules providing the means to chemically design molecules for quantum technologies. In a recently submitted paper, **XINXIAN CHEN** identified a new quasiparticle (the bexcitons) and showed that the dynamics of open quantum systems can be exactly mapped to the interaction of the system

with the bexcitons. As you can see, it has been a fun and busy time!

Leopoldo Mejía, Antonio Garzón-Ramirez and Wenxiang Hu recently graduated from our PhD program. Leopoldo is now a postdoc at Berkeley working with Rabani, while Antonio is a postdoc at Northwestern with Tempelaar. In turn, Wenxiang decided to continue in industry and joined Amazon as a scientist. Postdoc Chang Woo Kim accepted a faculty position at Chonnam National University in Korea, after a very successful stay at Rochester. Rylee Neumann completed his senior thesis in the group modeling Raman spectroscopies and is now a scientist at Lincoln Labs. Junjie Wang completed his undergraduate research in the group and is now a graduate student at Northwestern University. Luis Sierra completed his summer research in the group as part of the iScholar program and has now started his PhD at Northwestern.

In terms of additions, the group is very excited to welcome Dr. **ROMAN KOROL** as a postdoc in the group. Roman recently completed his PhD at Caltech and brings tremendous expertise in quantum dynamics. At Rochester, he is pushing the limits of analog quantum simulation. Mr. **RISHABH DORA** recently joined the group as a PhD student after completing his BS-MS at IISER Bhopal. In the summer, we hosted Mr. Jhoan Fernández from Universidad del Valle as part of our prestigious iScholar program. During the summer Jhoan investigated many-body effects in laser-driven currents. In the summer, we also welcomed Mr. **DEREK CHIEN** as a Beckman scholar in the group. Derek is currently investigating self-assembly processes in Janus molecules.

VISHAL TIWARI was awarded the Robert and Marian Flaherty DeRight Fellowship, and presented his work on laser-dressed materials in the Gordon Research Conference (GRC) on Quantum Control of Light and Matter and the MPI-PKS meeting on Dynamical Control of Quantum Materials. He was also part of a collaborative effort published in *Nature Physics* to isolate Floquet replicas in quantum materials. Xinxian Chen's work on tensor network hierarchical equations of motion was selected as a talk in the Gordon Research Seminar on Quantum Control. Ignacio Gustin received the Esther-Conwell fellowship and also presented his work at this key GRC.

This last year, Ignacio Franco presented the work of the group at EXCON (Santa Fe), APS March meeting (Las Vegas), Canadian Chemistry Conference (Calgary), Photodynamics (Havana), and in many other places around the world. He also spent the Fall at the University of Toronto as a visiting professor.

In terms of teaching, Ignacio Franco continues to teach CHEM251: Physical Chemistry I and loves teaching quantum mechanics. Ignacio has also been teaching an advanced graduate course "Quantum Dynamics," that is designed to help students transition from an introductory graduate course in quantum mechanics to state-of-the-art research in quantum dynamics.

The group looks forward to a new year of teaching, research and service!

From L to R: Rishabh Dora, Ignacio Gustin, Derek Chien, Jhoan Fernández, Vishal Tiwari, Xinxian Chen, and Ignacio Franco

Alison J. Frontier

Professor of Chemistry

Ph.D. 1999, Columbia University

RESEARCH INTERESTS

Studies of novel pericyclic reactions, cationic rearrangements and stereoselective cyclization cascades, and their application to complex molecule synthesis. Interested in reactions that produce unusual, densely functionalized ring systems from simple precursors.

CONTACT

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Professor **ALISON FRONTIER**'s research program is focused on synthetic organic chemistry. Research directions being pursued in the lab include the study of novel pericyclic reactions, cationic rearrangements and stereoselective cyclization cascades, and their application to complex molecule synthesis. Projects focus on reactions that can produce unusual, densely functionalized ring systems from simple precursors, for rapid assembly of polycyclic structures found in rare natural products. The lab has identified several variants of the Nazarov cyclization since studies began in 2002, making it possible to synthesize highly substituted cyclopentanes with different substitution patterns. Their frustration with divinyl ketone precursors has taken them on a convoluted search for better ways to generate pentadienyl cation intermediates, a journey that has been long but fruitful. These efforts have intersected with our long-standing interest in general strategies for building polycyclic molecules with embedded quaternary carbons.

Most recently, the group has developed an iterative cyclization strategy that engages three simple precursors: an enyne, a carbonyl building block, and a halide ion, and produces a complex halocyclopentene in one or two synthetic operations. Over the past few years, the group has reported on mix-and-match sequences using aldehydes, ketones, enol ethers, acetals, amides, and imines in the role of the carbonyl building block, enabling synthesis of carbocyclic scaffolds as well as N-heterocyclic scaffolds, containing five-, six- and seven-membered rings. The iterative cyclizations involve alkynyl Prins reactions, halo-Nazarov electocyclizations, and other transformations of cationic intermediates. In addition to building this portfolio of cationic cascades, the group took a surprising turn into high-nitrogen chemistry, when a former student (**PATRICK CARUANA**, PhD '07) approached them with a reaction he had discovered during the course of his work at the Center for Bio/Molecular Science and Engineering in the Naval Research Laboratory. He performed the calculations, and the work was published *Inorganic Chemistry*.

Patrick believed his collaborator (Professor Davin Piercey, Purdue Energetics Research Center (PERC)) had executed a tetra-aza-Nazarov cyclization, and asked us to investigate the feasibility of this using DFT techniques. **CONNOR HOLT** (PhD '22) performed the calculations and published the work in *Inorganic Chemistry*.

JACKSON HERNANDEZ defended his PhD work, describing his work on cationic double annulation reactions and iterative cascades initiated by aza-alkynyl Prins cyclizations. Jackson has taken a position as Senior Research Scientist at Curia in Albany, NY.

ALEKSA MILOSAVLJEVIC, **PATRYCIA ZYBURA**, and **YUSUF IBRAHIM** all graduate students working toward the PhD, are investigating new iterative cyclization methods of building natural products and natural product-adjacent targets using the group's cyclization strategies. To round out the team, the group's recent undergraduates include: **MAXWELL HUGHES** ('23) now a PhD student at Vanderbilt, and **ERIKA CERNA ARROYO** ('23) who is currently applying to PhD programs in medicinal chemistry. **ALEXANDRA LAWRIE** ('24) and **JOSEPHINE MYUNG** ('24) are busy with their senior thesis work, exploring cascades that will deliver new types of heterocyclic scaffolds.

From L to R: Alexa Lawrie, Alison Frontier, Jackson Hernandez, Aleksa Milosavljevic, Patrycia Zybura and Yusuf Ibrahim.

Pengfei (Frank) Huo

Associate Professor of Chemistry — Ph.D. 2011, Boston University

RESEARCH INTERESTS

Develops new theoretical approaches to investigate chemical reactivities when they are enabled by intrinsically quantum mechanical behavior, which has shown promise in enabling new paradigms that will profoundly impact energy production.

CONTACT

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The **HUO** group is developing new quantum dynamics approaches and investigating new chemical reactivities enabled by intrinsic quantum mechanical behavior. A recent focus of the group is to investigate new chemical reactivities inside an optical cavity. The group has had wonderful and productive years, with various exciting news including one recently funded award from NSF, a new award from Air Force Office of Scientific Research, and a collaborative NSF grant, as well as 12 publications, numerous awards for group members, and new group members!

Dr. **DUNCAN BOSSION** (PhD University of Montpellier, France) and former graduate student **SUTIRTHA CHOWDHURY** teamed up and pushed the idea of non-adiabatic ring polymer molecular dynamics into a new era! Duncan figured out a mathematically rigorous way to map discrete electronic states into continuous phase space variables, using the language of Lie algebra and Lie group! Using this new framework, the group gained a new state-of-the-art approach to quantize particles as classical variables and accurately simulate the coupled dynamics among them! This results in three papers in a nice trilogy. After departing from our group, Duncan stayed at the University of Gothenburg for another year and he is now an Assistant Professor of Physics at the Université de Rennes, France. We'll for sure miss him!

Dr. **DEPING HU** (PhD, University of Chinese Academy of Sciences) derived the analytic expressions of the nuclear forces from the polariton states, and simulated the quantum dynamics using on-the-fly electronic structure calculations! Deping returned back to China and started his independent faculty position at the Beijing Normal University, Zhuhai. The group will be in touch for more exciting research!

Dr. **YIFAN LAI** (PhD, University of Michigan) joined the group as a postdoc scholar in August 2022. He obtained his PhD and had done nice work in quantum master equation approaches and investigated using polariton to change charge transfer kinetics. In our group, Yifan will collaborate with **TODD KRAUSS'** group (through a collaborative DOE grant) to understand fundamental photophysics of the polariton relaxation process.

WENXIAN YING is making a wonderful contribution to our continuous adventure on vibrational strong coupling (VSC) influenced polariton chemistry. He had simulated the vibrational polariton quantum dynamics using an exact simulation approach, and even provided an analytic expression to explain the mysterious resonance conditions that experimentalists observed. The group envision that this analytic theory will be the golden rule in VSC, just like Marcus theory for electron transfer.

ERIC KOESSLER continues to develop his new theoretical approach that can simulate cavity loss dynamics through a stochastic method, resulting in a published work in *J. Chem. Phys* in 2022. He is actively collaborating with experimentalists to simulate the photoluminescence signals and predict how forming polaritons will help to enhance charge transfer reactions!

BRADEN WEIGHT, a PhD Student in Physics, enjoyed doing chemistry in the group and developed a new method to compute polariton states and energies in molecule-cavity hybrid systems, with ab-initio details of molecules, so it won't be just a physicist's toy model. This is a collaborative work with the Krauss group through the CCI, which was published recently in J. *Phys. Chem. Lett.*

MIKE TAYLOR, a PhD Student in Optics, continues to enjoy gauge problems in quantum optics. Not only has he resolved the famous ambiguity in quantum optics, but he continues to resolve cavity mode truncation ambiguity which was published in *Optics Letter*. Now Mike is working on a new framework that describes periodic systems (2D materials) coupled to the optical cavity.

ELIOUS MANDAL is developing path-integral

quantum dynamics approaches to simulate non-linear optical spectra when coupling molecules with optical cavities. This is a collaboration with the Krauss and Vamivakas groups at UofR and the Cundiff group at the University of Michigan through a DOE collaborative grant. Elious has made impressive progress!

BEN CHANG, a PhD Student in Physics, is working on stimulating polariton relaxation and decoherence processes using exact quantum dynamics approaches. This will help the experimentalist to understand some fundamental questions related to the polariton photophysical processes. He is also working on the polariton transport process, where the hybrid exciton-photon moves much faster than the exciton, which will connect many ongoing experimental works in this area.

SEBASTIAN MONTILLO and **SANTANU PODDAR** joined the group as new graduate students. Sebastian was in the group back in 2019 as an iScholar student, so it is really exciting to have him back. Sebastian will work on understanding the fundamental mechanism of polariton chemistry under the collective coupling regime. Santanu will work on exploring polariton quantum dynamics in the reciprocal space and developing new quantum dynamics approaches.

The group also had the pleasure to work with undergraduates. In summer of 2022, they hosted **MATEO LONDOÑO** (iScholar, '22) from the Universidad del Valle, Colombia, to perform his summer research project. Mateo has explored a new formalism of treating cavity loss when it is strongly coupled to the molecules. They also have the pleasure of working with **RUDIN KRAJA** (CCI-REU, undergraduate from University of Texas, San Antonio) on polariton mediated electron transfer. In summer of 2022, they hosted **JOHN ALEJANDRO MONTILLA** (iScholar, '23), also from the Universidad del Valle, to conduct research on a tight-binding model of the light-matter couplings. Lastly, the group had the pleasure to have **JIALONG WANG** (UofR Chemistry, BS, '22) conduct thesis research in our group. Jialong is exploring new selectivities of the Diels-Alder reaction coupled to optical cavity, using ab-initio simulation method.

FRANK HUO was tenured in 2022 and he is continuously writing proposals! Frank is thrilled to receive support from the NSF Chemical Theory, Models, and Computational Methods division with a new grant. This will support the quantum dynamics method development project in the group, with creative ways to quantize various particles, like electrons, protons, and photons! Frank is also excited to secure an award from the Air Force Office of Scientific Research, supporting their investigations of collective molecule-cavity coupling dynamics using ab-initio on-the-fly simulation approaches! To make it even more exciting, the collaborative research between the Huo group and the Yihan Shao group (University of Oklahoma) is funded by NSF through the Office of Advanced Cyberinfrastructure, and which will enable the group to deliver an integrated software platform for simulating quantum dynamics of chemical reactions in the next 3 years!

Frank is also honored to be recognized as the Hirschfelder Visiting Scholar from the Theoretical Chemistry Institute, University of Wisconsin, Madison, "for his outstanding contributions to both quantum dynamics and quantum electrodynamics for the study of chemical reactivities". He enjoyed his week-long visit where he connected with many old friends and got a chance to meet a lot of new friends. The group looks forward to additional exciting and productive years!

Huo group at NERM, Rochester NY.

From L to R: Deping Hu, Wenxiang Ying, Arkajit Mandal, Elious Mondal, Sebastian Montillo, Duncan Bossion, Braden Weight, Mike Taylor, Frank Huo, Eric Koessler, Ben Chng.

William D. Jones

Charles F. Houghton Professor of Chemistry Ph.D. 1979, California Institute of Technology

RESEARCH INTERESTS

Studies transition metal organometallic compounds for the cleavage of strong carbon-element bonds, with synthesis, structure, and reactivity being integral components of each project.

CONTACT

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The **JONES** group continues their work in organometallic chemistry and catalysis. Both **IGNACIO CAMARERO** and **AURODEEP PANDA** continue their graduate studies. Two MS students graduated recently. **RYAN POHORENEC** finished his thesis studying rhenium-FOX complexes, and **YUEHENG SAM MIN** completed his thesis on the synthesis of several photoswitch derivatives for the Center for Quantum Electrodynamics for Selective Transformations (QuEST). Bill was able to return to the Freie Universität of Berlin to work in the lab of Professor Christian Müller for a continuation of his Humboldt Senior Research Award. (Christian was a postdoc with Bill in Rochester in 2001).

Bill stepped down as Associate Editor for the *Journal of the American Chemical Society* at the end of 2020 after 18 years. He gave talks at the University of Washington, the University of Göttingen (ISCHA), and the Free University of Berlin. He also spoke at the International Symposium on Organometallic Chemistry in Prague, and ACS Meetings in San Diego and Chicago, and at NERM in Rochester. He also spoke at the Nichols Symposium celebrating the award given to Karen Goldberg. At the San Francisco ACS meeting in August, Bill was honored by a Symposium on Strong Bond Activation and a reception and dinner to celebrate his 70th birthday (in Oct. '23).

The group's scientific accomplishments have centered upon their work in amine and alcohol dehydrogenation, and in new dehydration catalysis. The group found an iron catalyst that could electrochemically dehydrogenate alcohols to ketones. This work is being extended currently to amine dehydrogenation to make imines. We are also engaged in synthesizing a series of new hindered metal-hydroxides for use in the Guerbet process to convert ethanol selectively to n-butanol. Here, ethanol is dehydrogenated to acetaldehyde, which then undergoes an Aldol condensation with itself to produce an α,β-unsaturated aldehyde. Rehydrogenation gives butanol, with water as the only byproduct. They have found a very selective tandem catalyst system that gives only n-butanol but no higher Guerbet products (products resulting from butanol reacting in a similar fashion with itself or with ethanol). They are also continuing to develop new chemistry with a class of fused-bisoxazolidine (FOX) ligands bound to first-row metals. In particular, our initial work focused on an iron-FOX complexes that could convert phenylethanol into styrene plus water in >70% yield. More recent work with a copper(II)FOX catalyst shows conversions to 98% styrene using toluene as solvent. Water separates from toluene and drives the dehydration to completion. Other applications of this catalyst are under development. Bill also has

a collaboration with Tulay Atesin at UT-RGV and has worked with several MS students on DFT calculations of C-CN activation in fluorobenzonitriles.

Bill also served on the International Advisory Boards for the ICOMC and ISCHA conferences. These meetings were held in Prague, Czech Republic, and Göttingen, Germany. The group is supported by continuing funding from the Department of Energy and the National Science Foundation.

Bill's grandsons, Henry and Charlie Simson, are now 8 and 5 years old, respectively. Both boys are doing very well, and Heather and Bill are delighted to see them often since they live in Rochester near Sea Breeze. Their son Simon and wife Danielle have a 2-year old daughter Madison, and they are able to visit them in Jersey City a few times a year. Their daughter Elizabeth and her husband Josh Sweet a have new dog in their family, and they live in Chili.

2023, Fairport, NY
Adults: Danielle & Simon Jones; Bill Jones; Elizabeth Sweet; Heather Jones; Josh Sweet; Sarah & Mike Simson
Children: Madison Jones; Charlie & Henry Simson

C. Rose Kennedy

Assistant Professor of Chemistry

Ph.D. 2017, Harvard University

RESEARCH INTERESTS

Synthetic and mechanistic catalysis, organometallic chemistry, and organic chemistry with an emphasis on human health and sustainability

CONTACT

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ROSE KENNEDY joined the Chemistry faculty in January 2020. Rose is an alumna of the Department, having earned a BS in chemistry from the University of Rochester in 2011, where she performed research under the guidance of Professors Kara Bren and Alison Frontier. Rose then completed her doctoral studies as an NSF Graduate Research Fellow with Professor Eric Jacobsen at Harvard University. During her time in the Jacobsen group, she elucidated key mechanistic features of ion-binding organocatalysis and introduced a synergistic ion-binding strategy for enantioselective catalysis. After defending her PhD in December 2016, Rose undertook postdoctoral research with Professor Paul Chirik at Princeton University, earning NIH NRSA Postdoctoral Research Fellowship support. At Princeton, she leveraged mechanistic insights to develop several iron-catalyzed methods for upgrading unactivated olefins through the formation and control of metallacyclic intermediates.

Rose is thrilled to have returned to the University of Rochester to launch her independent career as an Assistant Professor in the Department of Chemistry. In addition to innovating in research, Rose is passionate about teaching and promoting diversity & inclusion in STEM. In the spirit of Meliora, she is excited to continue advancing all three of these intersecting aims through her work in the University of Rochester chemistry community!

The Kennedy group is broadly interested in research challenges at the interface of synthetic organic and organometallic chemistry and catalysis. The group has been off to a strong start with a talented team of five graduate students and postdoctoral scholar Dr. **ABHISHEK KADAM** (PhD, Iowa State University) leading the way. **MEDINA AFANDIYEVA**, Abhishek, and undergraduate **XIJUE WU** ('23; Take-5, '24) have been leading the way in the design of bioinspired ligands for transition metal catalysts that activate complex reagents in a cooperative fashion. Abhishek, **HAILEMARIAM MITIKU**, and undergraduate **REBECCA REAGAN** ('24) have extended these designs to multimetallic systems for small-molecule activation. **VIVEK PILLAI**, and **KAYCIE MALYK** have been laying the mechanistic groundwork to achieve selective coupling reactions with biologically abundant motifs, and **DANIEL AKUAMOAH** has been applying those insights to new synthetic methodologies. We have begun to publish our initial progress in each of these areas (see above and stay tuned for updates!) and have secured our first grants to support this work from the ACS Petroleum Research Fund, the David and Lucile Packard Foundation, and the National Institute of Health.

Over the summers, we have hosted visiting reseachers through the iScholar and REU programs. In 2022, we welcomed **JORGE VALENCIA CASTAÑOS** from the Universidad del Valle in Colombia; Jorge subsequently started his PhD at the University of Pennsylvania. In 2023, we welcomed **JULIA SHOEMAKER** from Ursinus College in Pennsylvania; she's now finishing up her senior year at Ursinus. In 2023, University of Rochester undergraduate **WINIFRED DORLEAN** ('24) also earned a prestigious McNair Fellowship to support her research through the Spring and Summer. In Fall 2023, we've added two new undergraduate students to our team, **ABRAHAM ELLENBOGEN** ('25) and **MATTHEW GLEASON** ('26). We are also grateful to our undergraduate thesis alumni **SARAH CRAIG** ('21), **DALTON HANAWAY** (BS '21/MS '22), **ELLIOT SILK** ('22), and **DANIEL NAKAMURA** ('23). Sarah, Elliot, and Daniel are continuing to pursue their passion for chemistry research in PhD programs at the University of Pittsburgh, New York University, and Cornell University, respectively. Dalton is now working at a tech startup called Arch.

Kennedy group graduate and undergraduate mentees have also been recognized for their outstanding work with numerous awards. Medina, Vivek, and Daniel all

earned departmental fellowships over the past several years, and Medina also earned the prestigious Elon Huntington Hooker Fellowship to support her research in the 2023-2024 academic year. Medina and Abhishek were both recently recognized by the ACS for their leadership and excellence in Diversity, Equity, Inclusion, & Respect (DEIR) and in Mentoring, respectively. Sarah, Dalton, and Elliot all earned Dean Marvin Summer Research fellowships, and Elliot, Xijue, and Rebecca earned Discover Grants to support full-time independent research over the summers. Sarah and Xijue were both recognized for their outstanding ability and achievement in the field of science with Catherine Block Memorial Fund Prizes in their junior years, and Xijue also earned the Janet Howell Clark Prize in her senior year. Daniel Nakamura earned a research fellowship from the National Science Foundation to support his graduate studies at Cornell. The group is so proud of the accomplishments of every member–past, present, and future–of the team!

Follow the group on LinkedIn (https://www.linkedin.com/groups/12873442/) or online (https://www.sas.rochester.edu/chm/groups/kennedy/) to stay up-to-date on all the latest and greatest news!

2023 Commencement celebrations with Daniel Nakamura (BS '23), Prof. Rose Kennedy, and Xijue (Jade) Wu

Kennedy lab members in Fall 2023. Back row (L to R): Xijue (Jade) Wu, Matthew (Matt) Gleason, Vivek G. Pillai, Hailemariam (Haile) Mitiku, Daniel Akuamoah, Prof. Rose Kennedy.
Front row (L to R): Abraham (Abe) Ellenbogen, Rebecca Reagan, Kaycie Malyk, Medina Afandiyeva, Dr. Abhishek Kadam

Kathryn Knowles

Associate Professor of Chemistry

Ph.D. 2013, Northwestern University

RESEARCH INTERESTS

Synthesis and development of colloidal nanocrystals and nanostructured thin films of mixed-metal oxide semiconductors, electrochemical and photoelectrochemical studies of nanostructured oxide electrodes, time-resolved optical spectroscopy of nanomaterials.

CONTACT

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The **KNOWLES** group progressed through several significant milestones since the last newsletter update. After saying goodbye to founding members **MEHRIN TARIQ** and **DAVID BREWSTER** in 2021, four more members of the group joined the ranks of PhD alums of the Knowles group. **MELISSA KOCH** ('22 PhD) defended her PhD thesis describing electrochemical characterization of metal oxide nanomaterials in September 2022 and started a position as a Senior Scientist at Integer Holdings Corporation in Clarence, NY, shortly thereafter. **BRITTNEY BEIDELMAN** ('22 PhD) became the first group member to complete a PhD in Materials Science after she defended her thesis describing new methods to control the crystal phase of VO_2 nanocrystals in November 2022. She now works as a Principal Scientist in Materials at Luna Labs USA, LLC in Charlottesville, VA. **KARLA SÁNCHEZ-LIÉVANOS** ('23 PhD) defended her thesis describing the synthesis and photocatalytic properties of ternary spinel ferrite nanocrystals on Cinco de Mayo 2023. Karla is now a postdoctoral fellow at the RENEW Institute at the University at Buffalo supported by a prestigious NSF MPS-Ascend Postdoctoral Fellowship! **JACOB SHELTON** ('24 PhD) defended his thesis describing the polaromic optical properties of hemitite and is now a postdoc fellow at the National Renewable Energy Laboratory. Finally, **JAMES STAIR** ('21 MS) left the group this summer to start a position as a Laboratory Technical Associate with the Environmental Health and Safety Office at the University of Rochester.

L to R: Revathy Rajan, Erica Craddock, Jacob Shelton, Karla Sanchez-Lievanos, James Stair, and Katie Knowles

The group also has several graduations to catch up on among the undergraduate students. **XIAOTIAN ZHANG** ('23 BS) completed their senior thesis on the synthesis of VO_2 nanocrystals and started in the chemistry PhD program at Brown University. **TONG "MOLLY" SUN** ('23 BS) finished her senior thesis on the photocatalytic activity of ternary spinel oxide nanocrystals and will stay for an additional year to complete her MS degree in the group. Tian and Molly join other recent undergraduate alums including **DOMINICK SARAPPA** ('18 BS, '19 MS, now working at Reckitt in New Jersey), **YIFENG BIAN** ('19 BS, now at Clinical Laboratory Technologies at Labcorp in St. Paul, MN), **GARRETT HOTELING** ('19 BS, now a PhD student in chemistry at Colorado State University), **ANNABEL SELINO** ('20 BS, now a PhD student in chemistry at Cornell University), and **HANNAH ROBERTS** ('21 BA, now a Production Chemist at Interprint Group in Pittsfield, MA). In addition to these UofR undergraduates, the group has also had the pleasure of hosting several

summer students from elsewhere in recent years. These include **SINA WREDE** ('19 iScholar) from Sweden, **FRANCESCA ELVERSON** ('21 iScholar) from the U.K., **MARYAGNES BALOGUN** ('22 REU) from Morgan State University, and **MADDY WAHL** ('23 REU) from the Catholic University of America.

Along with these graduations, several students have joined the group. **ERICA CRADDOCK** and **REVATHY RAJAN** joined in December 2021 as PhD students in chemistry. Both Erica and Revathy successfully passed their qualifying exams and advanced to PhD candidacy in June 2023! **AIDA GUEYE** joined the group as a PhD student from the Materials Science program in December 2022. She successfully completed her first-year oral exam in the Spring of 2023! Erica, Revathy, and Aida are joined by **ELISE GENDRICH** ('24 T5), who will remain in the group to complete their senior thesis during the 2023-2024 academic year. **FRANKLIN XU** ('24) is a biology major currently keeping the Cu_2O catalysis project Mehrin started alive, and **SUBHAJYOTI MANDAL** joined the group in 2024.

They are proud to report that several group members recently earned recognition for their outstanding work. Karla Sanchez-Lievanos earned a department travel award and Carl Storm Fellowship to support her travel to Switzerland to present her work in the 2022 Gordon Research Symposium and Conference on Colloidal Semiconductor Nanocrystals. She also led the UofR team that wrote a successful proposal to organize a graduate student-led symposium at ACS in Fall 2022, earned the Elon Huntington Hooker Fellowship and Outstanding Graduate Student Award in 2021, and was named a 2023 CAS Future Leader! Brittney Beidelman earned the ACS Bridge Travel and Professional Development Award to support her attendance at the Fall 2022 ACS meeting in Chicago where she gave a talk about her work. Erica Craddock earned a W.D. Walters Teaching Award in 2022 in recognition of her outstanding work as a teaching assistant for the upper-level physical chemistry labs CHEM 231 and 232. Revathy Rajan earned a Sherman-Clarke Fellowship in recognition of her outstanding academic achievements during her first year of graduate school. Tian earned the ACS Award in Inorganic Chemistry in 2023. Other group members who earned awards since the last newsletter update include Mehrin Tariq (Department Travel Award in 2020), David Brewster (W. D. Walters Teaching Award in 2019 and DOE Graduate Student Research Award in 2020), Melissa Koch (W. D. Walters Award in 2020), Jacob Shelton (Esther M. Conwell Graduate Fellowship and NSF GRFP Honorable Mention in 2019, Elliot and Laura Richman Fellowship in 2020), Garrett Hoteling (ACS Award in Inorganic Chemistry in 2019), and Hannah Roberts (Chemistry Department Award in 2021).

Over the past few years, Katie has been named a Scialog Fellow in Negative Emissions Sciences and a recipient of the NSF CAREER Award. More recently, Katie was promoted to Associate Professor with Tenure effective July 2023! This incredible accomplishment recognizes the hard work and achievements of all current and former members of the Knowles group. Thank you all for your contributions!

Katie and JC with their children Leo and Willa

Todd D. Krauss

Professor of Chemistry

Ph.D. 1998, Cornell University

RESEARCH INTERESTS

Physical chemistry; synthesis and characterization of nanometer scale materials and devices with relevance for renewable energy, techniques include single molecule photoluminescence spectroscopy, atomic force microscopy, ultrafast and nonlinear optical spectroscopy. Biophysical chemistry; quantum optics and strong light-matter coupling.

CONTACT

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Lots has happened in the **KRAUSS** group since the last update pre-COVID. Most importantly, they had **JENNIFER URBAN, TREVOR TUMIEL, JULIE SMYDER, ABBY FREYER, BECKAH BURKE**, and **NICOLE COGAN** all receive their PhD degrees! Congrats to all! **KEVIN MCCLELLAND** came back for a postdoc and has since left to take an industrial position as a productive member of society. **WESLEY CHIANG** joined the group and got his Masters' Degree, and then rejoined as a biophysics PhD student a few months later. **KAELYN MCFARLANE-CONNELLY**, **AIDEN OI**, and **CALEB WHITTIER** all did senior thesis projects with the group and subsequently went on to graduate school in Chemistry.

In the last couple of years, the group had a fair amount of success in obtaining funding for several new research directions, meaning that what the group is working on looks a lot different in many respects than pre-COVID. In terms of current graduate students in the group, establishing structure-function relationships between optical and charge properties in carbon nanotubes and colloidal CdSe nanoplatelets using the atomic force microscope (AFM) is **ERIN CHRISTENSEN,** continuing the group's long history of pushing the limits of what an AFM can measure. **WES CHIANG** is making virus-like nanoparticles containing CdSe quantum dots in order to understand the biochemical origins of long neuro-COVID. This is a relatively new research direction done in collaboration with Dr. Handy Gelbard from URMC. **OVISHEK MORSHED, BEN HANCOCK, JIAHUI WEI,** and **MITESH AMIN** are all looking at various aspects of strongly coupled light-matter systems, pushing them deep into quantum optics as applied to nanomolecular systems. Specifically, they are placing assemblies of CdSe nanoplatelets inside of optical cavities where the cavity optical modes are in resonance with the exciton absorption of the nanoplatelets, forming an excitation called a polariton. Ovishek and Jiahui have focused on cavity fabrication and characterization, and Mitesh on polariton photophysical dynamics. Ben wants to take the project in a challenging direction: chiral optical cavities. The group has also expanded their research related to the photocatalytic production of hydrogen from sunlight, which now includes **LIZ PHINNEY**, **FARWA AWAN,** and **CHAYAN CARMENATE-RODRIGUEZ**. Liz is working on new types of nanoparticles for catalysis, and Chayan is our ultrafast spectroscopist measuring charge transfer

The Krauss Group

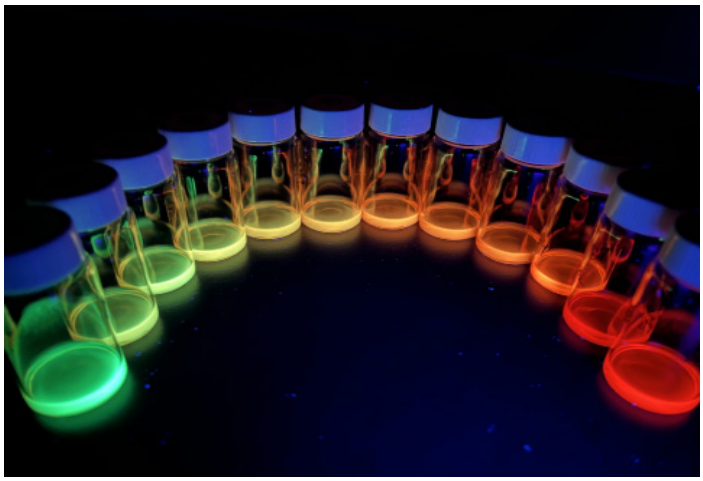
A group reunion

rates. Farwa is part of a new project that is exploring the use of machine learning to better understand and maximize photocatalytic rates and efficiencies. **WILLIE GIRTEN** received a DOE fellowship (congrats Willie!) to study at the National Renewal Energy Laboratory for 9 months starting in November 2023. Willie researched why the use of chiral ligands on CdSe nanoplatelets leads to a chiral-optical response with respect to the absorption of light.

Several newcomers joined the group for the fall of 2023 including the new postdoc Dr. **APURBA DE**, who is going to build a coherent multidimensional spectroscopy setup using the newly purchased amplified fiber laser (i.e. the "Death Star"). **JENNY YAO** and **PAUL BLOOM** are undergraduate students who are getting their first taste of nanoscience research in the laboratory. Jenny is working on nanoplatelet synthesis, while Paul is studying the fabrication of new optical cavities.

After 9 years, **TODD KRAUSS** stepped down from Department Chair in 2022 – rejoining the "rank and file" faculty. However, no rest for the weary as the group was fortunate to be awarded an NSF Phase I Chemical Innovation Center grant in 2021, with Todd as a PI. This is a multi-PI and multi-institutional center grant which has kept Todd quite busy administratively speaking, with the Phase II proposal submitted in October 2023. They were also very excited to have the first Krauss Group Reunion! Many thanks to Erin Christensen, Trevor Tumiel, Katie Leach and Lisa Nogaj (nee Carlson) who helped to organize the event, and thanks to all who made the trip back to Rochester. It was great to see everyone again!

If you want to keep current with the Krauss group comings and goings – they are on X (formerly known as Twitter). X-heet them at @KraussLabUR. And don't forget that Lisa Carlson Nogaj and Katie Leach put together a Facebook page for the Krauss group! They want to use it to stay in touch with current members and alums – and they want to get current updates from former Krauss group members! https://www.facebook.com/groups/kraussgroup/. Have a great year!



Ellen Matson

Marshall D. Gates, Jr. Professor of Chemistry — Ph.D. 2013, Purdue University

RESEARCH INTERESTS

The synthesis, characterization, and multielectron reactivity of metal-chalcogenide clusters and actinide complexes, with the goal of developing new strategies for storing renewable power through its conversion to electrochemical energy and chemical fuels. Our group works in four distinct research areas: (1) modelling the surface chemistry and reactivity of reducible metal oxides; (2) engineering of nanoscopic molecular charge carriers for redox flow battery technologies; (3) the development of nanosystems for photocatalytic hydrogen generation; and (4) the investigation of the electronic structure of low-valent actinide complexes. **CONTACT**: matson@chem.rochester.edu

A lot has changed in the **MATSON** Laboratory since the last update. The group is composed of six graduate students and two postdocs! **SHANNON COONEY, MAMTA DAGAR, CHARI PETER, KATHRYN PROE,** and **LEYLA VALERIO** all successfully completed their cumulative and oral qualifying exams! Shannon, Chari, and Katie have been working diligently to understand hydrogen atom uptake and transfer at the surface of a family of polyoxovanadate-alkoxide clusters, each publishing their first papers on the topic during the past academic year! Mamta has been pioneering some new directions related to redox flow battery research in the lab, including a detailed electroanalysis of vanadium oxide assemblies, as well as elucidation of new molecular charge carriers for energy storage technologies. Leyla's projects to date have focused on the photophysics of low-valent uranium complexes – her research pushes forward their understanding of the role of f-electrons and orbitals in excited state electronic structures of organometallic actinide complexes. In December 2022, they welcomed **BECCA WALLS** to the research team. This fabulous group of women

Matson Group, Spring 2023

mat n lab

synthesis for energy storage and conversion

is pushing the boundaries of inorganic synthesis and photo/electro chemistry. Their boundless creativity and fearless approach to research have launched a number of new and exciting projects in the group!

In January of 2023, the Matson Lab welcomed two new postdoctoral researchers, **ZHOU LU** (PhD, University of North Texas) and **KAMALESS PATRA** (PhD, IIT Kanpur). Both have taken on new research projects in the group, expanding the group's expertise in metal chalcogenide clusters. They look forward to sharing their work in a series of exciting publications in 2024!

The graduate students in the Matson Lab have continued to collect numerous awards! In the 2022-2023 academic year, **ERIC SCHREIBER** (PhD, 2023) was named the recipient of both the prestigious University of Rochester Messersmith Fellowship and the 2022 Department of Chemistry Outstanding Graduate Student Award. Chari and Shannon were both selected as recipients of the W. D. Walters Teaching Award, an accolade given to graduate students who have demonstrated excellence in undergraduate education. Mamta's excellence in academics and research was recognized with her receipt of the Department of Chemistry Sherman Clarke Fellowship. Finally, Leyla received word in April of her receipt of a Graduate Fellowship from the National Science Foundation, a recognition given to some of the most promising graduate students from across the country!

Undergraduate research in the Matson laboratory has continued to thrive. **THOMPSON MARINHO** ('23) continued his research activities in the Summer of 2023, investigating the synthesis of oxidized

forms of polyoxovanadate-alkoxide clusters. **ERIN STOCKDALE** ('24) spent her summer working with our actinide subgroup, targeting improved understandings of the synthesis and electronic structure of some new low-valent uranium complexes. **DANIEL KESSLER** ('25) and **MOLLY CORR** ('24) continued their synthetic efforts toward the identification of soluble, titanium-substituted polyoxovanadate-alkoxide clusters, targeting energy-dense materials for next-generation redox flow battery technologies. Recently, the group welcomed two new undergraduate researchers, **ALLEN WANG** ('24) and **JOSHUA MCPHERSON** ('24). The group is excited to see what they accomplish as they continue their research into the academic year!

LAUREN VANGELDER (PhD 2019) works as an Assistant Professor at Norfolk State University and recently received the Students' Choice Professor of the Year Award. This past spring, Lauren graduated her first cohort of undergraduate students with degrees in chemistry!

After completing a postdoctoral position at National Renewable Energy Laboratory, **BRITTNEY PETEL** (PhD 2020) has taken a job at Starfire Energy working as a materials scientist. **RACHEL MEYER** (PhD 2021) works as a postdoctoral researcher at Berkeley with Polly Arnold. Rachel has been an integral part of establishing the Arnold Lab at the Lawrence Berkeley Laboratory, and is in the process of submitting her first manuscript! **ALEX FERTIG** (PhD 2022) works in Dayton, Ohio, for Faraday Technologies. In his role as senior scientist, he has participated in writing successful grants for government and commercial projects. After graduating in May 2023, **ERIC SCHREIBER** (PhD 2023) started a postdoctoral position in the laboratory of Amymarie Bartholomew at Yale University.

For **ELLEN MATSON**, 2022-2023 was another busy academic year, filled with talking, travelling, and teaching. Ellen was promoted to Associate Professor in July of 2021 – she enjoyed her first years of her tenured existence! In the Fall of 2022, Ellen had the opportunity to present the Kavli Emerging Leader in Chemistry lecture at the ACS National Meeting. Learn more about research in charge compensation and transfer at vanadium oxide surfaces in her recorded lecture here: https://www.acs.org/meetings/acs-meetings/past-meetings/kavli-lecture-series.html.

The Matson-Hicks family also had a banner year! Tad Hicks started school; his outgoing personality and knowledge of all things "squid" took Dudley Elementary School by storm. He's developed a passion for soccer, Pokémon, and his neighborhood squad. Lina Hicks took her first steps, and has since blossomed into a full-fledged toddler! She is obsessed with her baby doll, stuffed animals, and any object with which her brother is actively playing. Scott and Ellen celebrated 10 years of marriage and continue to be in awe of the little people in their home.

Follow them on Twitter (@MatsonLab) or check out the group's website (www.ellenmatsonlab.com) to stay up- to-date on the latest developments!

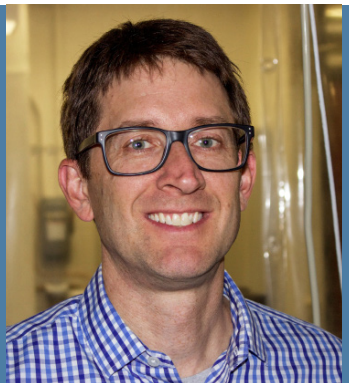
L to R: Chari Peter, Mamta Dagar, Katie Proe, Leyla Valerio, and Shannon Cooney pass their cumulative and oral examinations

Alex (left) and Eric (right) are hooded at commencement.

David W. McCamant

Associate Professor of Chemistry

Ph.D. 2004, University of California, Berkeley



RESEARCH INTERESTS

Ultrafast vibrational spectroscopy of structural dynamics in photochemistry; vibrational coupling and relaxation; structural rearrangements and relaxation mechanisms in photoexcited nucleic acids; Ultrafast energy and electron transfer processes relevant for solar energy systems.

CONTACT

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DAVID MCCAMANT has had a fun and stable group through the whole COVID era and into 2023. **STEVEN DIAZ** has been their senior student, developing femtosecond stimulated Raman spectroscopy (FSRS) of opaque scattering samples. Steven graduated in August and has started a postdoc at the University of Minnesota working with Professor Renée Frontiera. **JUAN SANDOVAL** joined the group in 2019 and has taken on the challenging theoretical work of explaining the vibronic states of exciton coupled J and H dimers. Juan has also developed methods that use the resonance Raman spectrum to test how well different DFT functionals predict the shape of excited state potential energy surfaces. **LIKUN CAI**, the group's Materials Science PhD student, has been pursuing varied projects, initially developing new calibration methods for solar hydrogen production measurements and, recently, testing the performance of different sensitizers in photoinduced electron transfer reactions on both p-type and n-type semiconductors. Brendan Courtsal did his undergraduate senior research in their lab before getting his BS in 2020 and then transitioned to the graduate program completing his MS degree in 2023. Brendan did a huge number of steady state measurements to establish the equilibrium constants for dye aggregation, values that are critical for Juan's studies being published.

Dave has been enjoying teaching CHEM231: Chemical Instrumentation, and CHEM232: Molecular Spectroscopy. He is continuing to lead the Department's REU program and was the programming chair for the North East Regional Meeting of the American Chemical Society (NERM 2022), which was held in Rochester in October 2022. (Finally! After 5 years of planning including a 2-year delay due to the pandemic.)

Professor McCamant and student Ellie Vetack during an awards ceremony.

Bradley L. Nilsson

Associate Professor of Chemistry

Ph.D. 2003, University of Wisconsin, Madison

RESEARCH INTERESTS

Bioorganic chemistry and chemical biology; amyloid peptide self-assembly; Alzheimer's disease; amyloid-inspired materials, HIV infectivity and microbicide development.

CONTACT

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The last year has been an eventful one in the **NILSSON** group. Students, both graduate and undergraduate, have completed their studies at the University of Rochester and have moved on to new positions. Current graduate students have progressed in their work and are advancing towards completion of PhD degrees soon, and they have welcomed new students into the group.

Recent former students have found positions in industry. **BRITTANY ABRAHAM** (MS 2019, PhD 2022) completed her postdoctoral research with Professor Danielle Benoit (Biomedical Engineering, University of Rochester) and joined iuvo BioScience (Rush, NY) as a Scientist in their Medical and Diagnostic Laboratories.

ELENA QUIGLEY (MS 2019) accepted a position at Alvogen/Norwich Pharmaceuticals (Norwich, NY). The group is confident that Brittany and Elena will find great success in their current work!

MELISSA JAGROSSE (MS 2020, PhD 2022) completed her PhD studies. She successfully defended her PhD thesis, "New Biomaterials for the Functional Delivery of Biological Macromolecules," in November 2022. Her work in the development of supramolecular hydrogel biomaterials for the sustained release and delivery of protein therapeutics was recently published (*ACS Biomaterials Science & Engineering*, 2023, 9, 784–786), and another manuscript based on her work on the mechanism of action of cyclic peptide agents used in the cellular delivery of siRNA was recently accepted for publication (*Molecular Pharmaceutics* 2023, 20, DOI: 10.1021/acs.molpharmaceut.3c00455). She was also a key contributor to a patent application based on her work on the development of low molecular weight agents for the functional delivery of siRNA to cells ("Amino Acid Derivatives as Novel Delivery Agents for Functional Delivery of Oligonucleotides", Provisional Application for Letters Patent, U.S. Application No. 63/422,967, November 2, 2022). Melissa has now joined Alexion Pharmaceuticals in the Rare Disease Unit of Astra Zeneca (New Haven, CT) as a Research Scientist. She is enjoying her work in the pharmaceutical industry.

FRANCINE YANCHIK-SLADE successfully defended her PhD thesis in January 2024. She participated in a collaborative research project with Marc Halterman, Craig Morrell, and Scott Cameron of the University of Rochester Medical Center using functionalized magnetic nanoparticles to model ischemic stroke in mice. In addition, she has also worked on understanding peptide self-assembly phenomena in which enantiomeric peptides coassemble into novel rippled beta-sheets. She accepted a position as a Technical Mass Spectroscopy Specialist at Shimadzu Scientific Instruments (Columbia, MD). She is a contributing author on a recent publication in collaboration with the groups of Professors Todd Krauss and Handy Gelbard (*ACS Applied Nano Materials* 2023, 6, 15094–15107).

HANNAH DISTAFFEN (MS 2021) has had a successful year and is making rapid progress in her Ph.D. thesis research. She is working to understand the pleated and rippled beta-sheet assembly of simple beta-sheet peptides and is also interrogating the interactions of these types of peptides with cell membranes to understand potential sources of cytotoxicity of amyloid systems. Both projects are in collaboration with Professor Cristiano Dias (Physics, New Jersey Institute of Technology). The Dias group is using computational molecular dynamics simulations to gain insight into these phenomena to both guide and explain the group's experimental efforts. Hannah is a contributing author on a recent manuscript describing membrane damage by amyloid peptides (*ACS Chemical Neuroscience* 2022, 13, 2766–2777). Hannah also presented this research at the 28th American Peptide Symposium (Scottdale, AZ; June 24–29, 2023). Her attendance at this meeting was supported by travel awards from the Department of Chemistry and from the American Peptide Society.

CHRIS JONES (MS 2021) has also made significant advances in his PhD research. His contributions to their

work in the development of cyclic peptides for siRNA delivery was recognized with coauthorship on a recently accepted manuscript (*Molecular Pharmaceutics* 2023, 20, DOI: 10.1021/acs.molpharmaceut.3c00455). Chris has also made interesting discoveries in understanding the coassembly of peptides of opposite stereochemistry into rippled beta-sheets. He is at the forefront of new collaborative work funded by the National Science Foundation where they are working with Professor Edward Egelman (University of Virginia) to structurally characterize these assemblies using cryo-EM techniques. They are extremely excited about this work. Chris also presented his work at the 28th American Peptide Symposium this last summer (Scottdale, AZ; June 24–29, 2023).

PAMELA AGREDO joined the Nilsson Group as a new graduate student in Fall 2021. She made rapid progress on her work in the study of novel supramolecular hydrogel biomaterials during her first several years in the Nilsson group and contributed as a coauthor on several published manuscripts (Langmuir 2022, 38, 15494–15505; *ACS Biomaterials Science & Engineering*, 2023, 9, 784–786). Unfortunately for the Nilsson group, Pamela moved to UT Dallas this summer with her husband, a member of the Fasan group, and will complete her PhD studies in Texas. The group will miss her but are confident of her continued success!

RITTY MOHAN, a former Fasan group member, joined the Nilsson group and has been an excellent addition to the lab. She is making rapid progress in her research during the first months of her time in the Nilsson lab, and they feel fortunate to have her as a new group member!

The Nilsson group has continued to benefit from the work of excellent undergraduate research students. Undergraduates in the Nilsson group include **JINGFEI DAI, SYDNEY CARTER, ZACHARY SCHREMMER,** and **IAN ARNOLD**. Several undergraduate researchers have recently completed their studies at the University of Rochester and have moved on to graduate studies elsewhere. These students include **JULIAN VON HOFE** (2022) (New York University, Chemistry), **CLAUDIA GARCÍA** (2023) (Tulane University, Biomedical Engineering), **YAHUI GUO** (2023) (Boston University, Chemistry), and **LOREN CARDANI** (2023) (Columbia University, Chemistry). The group is proud of all their undergraduate students and will be watching them with great interest and confidence in their success.

The Nilsson Group

Shauna Paradine

Assistant Professor of Chemistry Ph.D. 2015, University of Illinois at Urbana-Champaign

RESEARCH INTERESTS

Organic Chemistry and Organometallic Chemistry

CONTACT

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2022-2023 was a big year for the **PARADINE** lab. Through the group's focus on advancing novel catalytic strategies for scaffold-building transformations to prepare sp3-rich organic scaffolds, they have established two distinct research areas in palladium catalysis and copper catalysis. They are starting to see the fruits of all the hard work that the early group put in, starting a research program from scratch and dealing with the challenges of a pandemic. This has included the first major funding for the group: they were awarded both the NSF CAREER award and NIH R35 MIRA this year, as well as an internal University Research Award. It's an exciting time for the young group!

This year, they welcomed new members and said goodbye to others. In Summer and Fall 2022, they welcomed two new undergraduate researchers, **PRISCILLA PETERS** ('25) and **JOSEPH DEROSA** ('25); Priscilla and **AIDAN KROPIWNICKI** ('23) were both awarded the Schwartz Discover grant to support their research in Summer 2022. Aidan graduated with a BS in chemistry in Spring 2023, heading off to Brown University to pursue his PhD in polymer chemistry. They also saw their first PhD graduations: **KAITLYN (KAIT) HOUGHTLING** in June 2023 and **JAKUB VAITH** in July 2023; Kait took a medicinal chemistry position at Southern Research in Birmingham, AL, and Jakub took a medicinal chemistry position at Hexagon Bio in South San Francisco, CA.

Celebrating the group's 1st JACS publication (L to R: Greg Spaulding, Shauna Paradine, Jakub Vaith, Dasha Rodina)

Students in the group were also recognized for their accomplishments: Aidan won a Chemistry Department Award, and Jakub won a 2022-2023 Hooker Fellowship, which he declined as he was also recognized with the Bristol Myers Squibb Graduate Fellowship in Synthetic Organic Chemistry, among the most prestigious national fellowships for senior graduate students in organic chemistry. Other group members were recognized with departmental graduate fellowships in Fall 2022: Kait, **DASHA RODINA,** and **OWEN MONTEFERRANTE.**

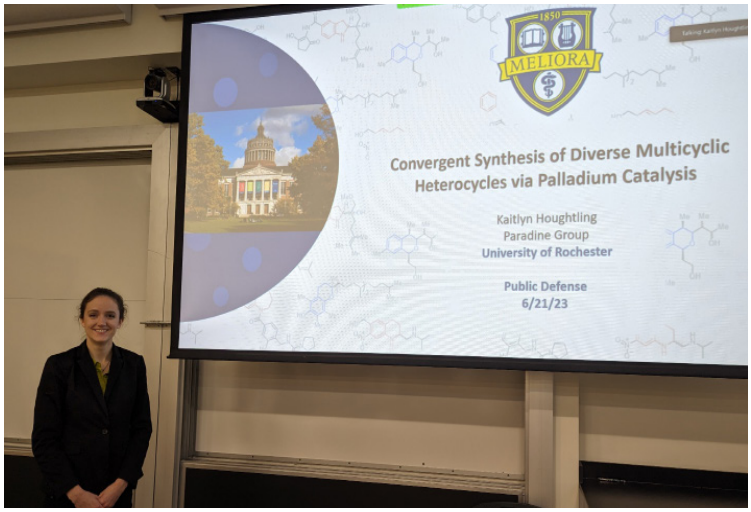
The group's first publications came out in *JACS* and *Organic Letters* in the Spring/Summer of 2022; their *JACS* paper (led by Jakub and Dasha), which described the establishment of ureas as a ligand platform for palladium catalysis, enabling the heteroannulation of dienes and bromoanilines to efficiently prepare indoline heterocycles, was among the most read papers in *JACS* for two months after its publication. Their *Organic Letters* paper, led by Kait and **AMANDA CANFIELD**, expanded the scope of their urea-enabled methodology to bromophenols, resulting in dihydrobenzofuran products. Since then, they have been applying these seminal discoveries in diverse directions, working toward their goal of establishing a unified strategy for the synthesis of diverse aliphatic heterocycles.

Spring 2023 saw the first paper from the group on oxidative copper catalysis; **CAITLYN (CAY) MCNICHOL** and **ETHAN DECICCO** led this effort together, supported by Amanda and former undergraduate **DANIEL CARSTAIRS** (BS '22). Cay and Ethan discovered an aerobic aminooxygenation reaction, which transformed cinnamyl N-alkoxycarbamates

into α-oxo-oxazolidinones in a single step under mild conditions – low copper loadings, room temperature, and using ambient air. Most excitingly, their mechanistic studies revealed that cooperative coordination of ligand and substrate to copper resulted in rapid reduction of Cu(II) to Cu(I), promoting oxygen activation and a free radical mechanism. This switch in mechanism from previous related methods opened up an entirely new substrate class for this transformation, and they're finding that this approach can be generalized to other oxidative, radical cyclization reactions.

The group has been taking full advantage of opportunities to advance themselves professionally – in Summer 2022, both Kait and Ethan were selected for internships at Pfizer through the Future Leaders Program. In Summer 2023, Dasha was awarded a DAAD-RISE Professional Internship at BASF in Ludwigshafen, Germany; Amanda interned at Merck Discovery in Boston, MA; and Cay interned at Seagen Pharmaceuticals in Seattle, WA. Ethan recently had a first-author paper published in *Organic Letters* based on his internship research, and Dasha, Cay, and Amanda are all likely to see papers from their internships as well. The group also got around to share their science, from ACS-NERM right here in Rochester, to the national ACS meetings (in Chicago, Indianapolis, and San Francisco), to GRC meetings (Heterocycles, in 2022 and 2023), to the International Conference on Heterocyclic Chemistry, and regional symposia as well.

They can't wait to see what the next year brings as their group continues to develop!



Right photo: The group's 1st PhD graduate, Kait Houghtling, preparing to give an outstanding final defense

Below: Paradine group, April 2023 (Front: Priscilla Peters, Ethan DeCicco, Dasha Rodina, Shauna Paradine, Amanda Canfield, Joe DeRosa; Back: Aidan Kropiwnicki, Owen Monteferrante, Shannon O'Neil, Jakub Vaith, Cay McNichol, Kait Houghtling)

Benjamin Partridge

Assistant Professor of Chemistry

Ph.D. 2018, University of Pennsylvania

RESEARCH INTERESTS

Develops supramolecular materials that mimic functional components of living systems. Current projects include designing adaptive capsules as protein chaperones and programming the assembly of proteins and nucleobases into fibrous materials.

CONTACT

benjamin.partridge@rochester.edu

This past year was a year of firsts for the **PARTRIDGE** group, which launched in the Chemistry Department in July 2022. Ben joined the department from a postdoctoral stint at Northwestern University, where he worked with Chad Mirkin on building protein-based materials using DNA. The Partridge group will focus on supramolecular chemistry–the study of how molecules come together to form larger assemblies–specifically leveraging noncovalent chemistry to design functional mimics of essential biological components from simple, synthetic building blocks.

Graduate student **LIZ PIEDMONT** joined the group on day one and immediately took the lead on developing self-assembling molecules that function as synthetic chaperones. Chaperones are ubiquitous proteins in natural cells and help other proteins to fold into their correct structures. When this process goes awry, unfolded proteins can assemble into toxic aggregates that have been implicated in conditions including Alzheimer's diseases, cataracts, and diabetes. Liz has been exploring a series of molecules, termed amphiphilic dendrons, for their ability to act as synthetic mimics of natural chaperones. Excitingly, Liz discovered that her molecules assemble in aqueous solutions and are able to reduce the extent of fibrillation of a model amyloid peptide fragment! This exciting initial study was submitted for publication in RSC Chemical Biology, and work continues apace to understand the molecular mechanism of the dendrons' inhibitory action.

The summer research team was quickly joined by incoming graduate student, **HANNAH CLAUS**, who officially joined the group after rotations in the Fall semester. Hannah is also working on the development of synthetic chaperones but is focusing on how the interactions between the group's synthetic dendrons and native peptides can be tuned using host-guest interactions and photoresponsive switches. To support her research, Hannah was selected as a trainee for the NIH T32 Chemistry-Biology Interface (CBI) Predoctoral Research Training Program, which will provide excellent interdisciplinary training opportunities beyond her work in the group. Hannah also launched our group's Twitter account (@PartridgeGroup).

THE PARTRIDGE GROUP

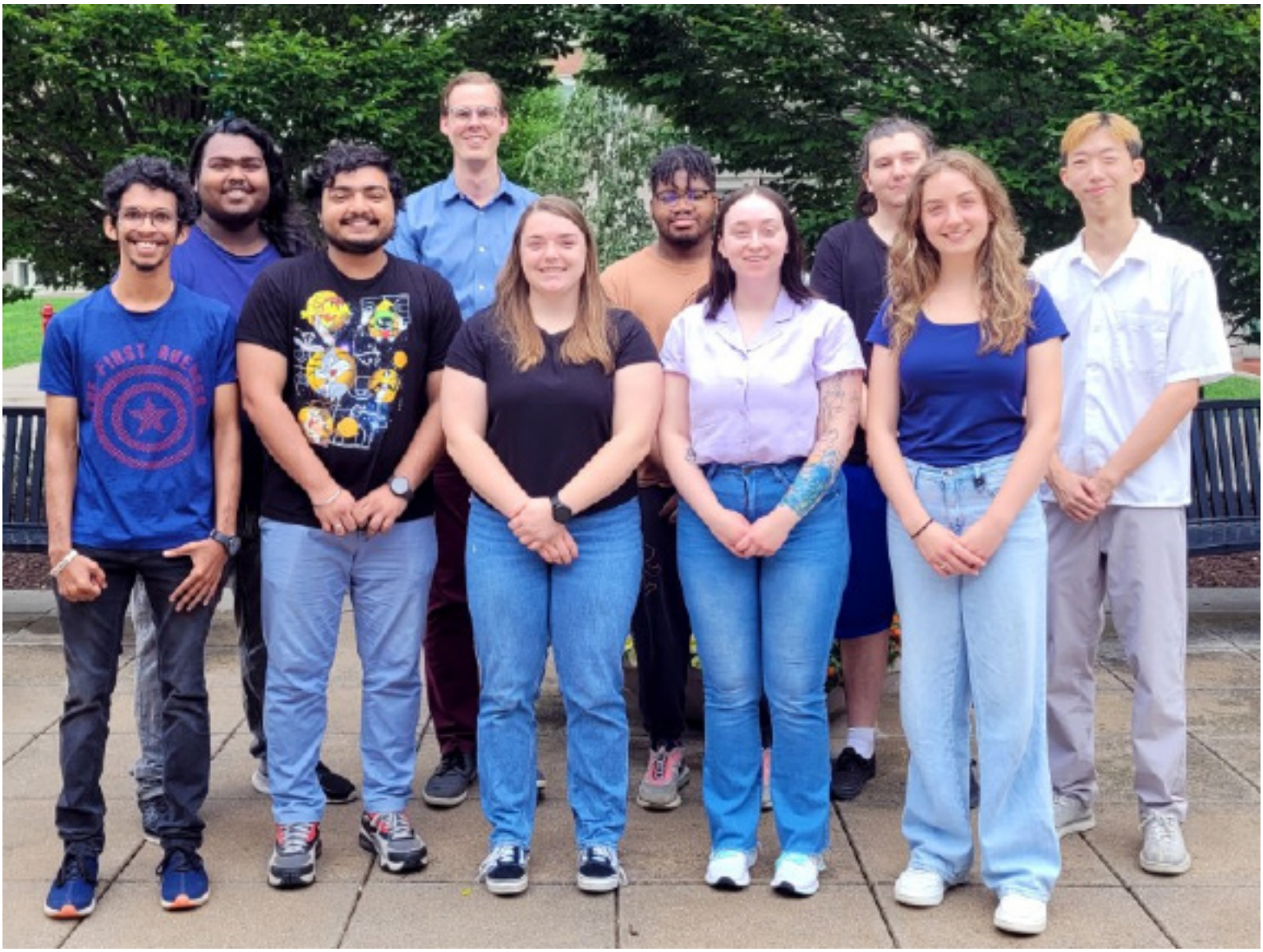
Two more graduate students joined the lab in the Spring semester: **ABHISHEK ROY** and **PARBHAT KUMAR**. Abhishek is developing photoresponsive analogues of GTP, a common enzyme cofactor, to enable synthetic control over natural protein assembly processes. Parbhat is focused on developing new bifacial nucleobases that can assemble into sequence-specific macrocycles as building blocks for hierarchical fibrous assembly. Both Abhishek and Parbhat received Sherman-Clarke Fellowships from the Department in recognition of their excellent academic performance in first year courses.

The group has also benefitted from the enthusiasm and expertise of several undergraduate students. **GRACE VAN DER MEER** ('25) and **CAMDEN PARKER** ('23) joined in July 2022 as Dean Marvin Summer Scholars and continued research throughout the academic year. Grace's research aims to control protein assembly via the design and installation of prosthetic photoswitches, while Camden was looking into an iterative synthesis of macrocyclic styrenes. Camden graduated in May 2023 and is now working as a chemist at FreshAir Sensor. In the Fall semester, **AIDEN WARD** and **UBANNI OPASHI** (both '25)

joined the group and are both developing novel bifacial nucleobases for supramolecular assembly. The group has had its first few crystal structures (with help from Bill Brennessel) and more are sure to come! Aiden and Ubanni were recognized with Schwartz Discover Grants from the Office of Undergraduate Research to support full-time research in Summer 2023, as was **MARVIN WU** ('26), who started work on the chaperone project with Liz. They also hosted a high school student, **NINA ZIMAKAS**, for a 10-day research experience in June.

The group has welcomed two international undergraduates through the Department's iScholar program, which Ben co-directed this year with Prof. Knowles. In Summer 2022, **ÁRON ADORJÁN** (Hungary) helped to establish the lab and the bifacial nucleobase project, while in Summer 2023, **BASIL BIJU ALIYAS** (India) picked up the baton and continued work on the nucleobase project, mentored by Parbhat. Áron has just started PhD studies with Tobias Ritter (Max-Planck-Institut für Kohlenforschung) and Basil is currently finishing his BS-MS degree.

The last year has flown by – it has been an exhilarating year in the group and they've assembled a fantastic team of students. They're excited to build on their momentum as they look forward. Watch this space!



The Partridge Group in Summer 2023. Back row (L to R): Abhishek Roy, Ben Partridge, Ubanni Opashi, Aiden Ward, Marvin Wu. Front row (L to R): Basil Biju Aliyas, Parbhat Kumar, Hannah Claus, Liz Piedmont, Grace van der Meer.

Lewis J. Rothberg

Professor of Chemistry

Ph.D. 1983, Harvard University

RESEARCH INTERESTS

Physical chemistry: photophysics of conjugated organic materials for solid-state lighting and solar energy conversion, metal nanoparticle-enhanced molecular spectroscopy, biomolecular sensing.

CONTACT

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LEWIS ROTHBERG's group has continued their work on interferometric sensing of biomolecular attachment with **FAKHRADDIN AKBARI DOURBASH** demonstrating successful detection of immunoglobulins and producing exciting initial results on nut allergens derived from real samples: peanut cookies from the vending machine purposely spiked with almond and/or cashew flour! On the strength of Fakhraddin's work, they obtained NSF joint funding with a small company, ELISA Technologies, to develop a portable sensor capable of determining whether meats have been contaminated. In the meantime, Fakhraddin was offered an outstanding job that is a great fit for his work at Sartorius in the Bay Area and has moved on. In his wake, a new graduate student **ZONGLUN LI** (Chemical Engineering) and a number of excellent undergraduates **ANDREW OPHARDT, MINHUI LIU, GEORGIA HOLLINGSWORTH** (Trumansburg State, REU), and **EMMA BELLIN** have stepped in and moved the project forward. The reflective interferometric method has attracted other collaborators, including Alex Shestopalov's group in Chemical Engineering, and they are exploring together its utility in studying real time growth kinetics for atomic layer epitaxy of various oxides on silicon. The group's organic electronics work also continues with a foray into studying stimulated emission in organic LEDs with Dr. Mitchell Nelson of Organophotonics, LLC. It has been fascinating to rediscover (and learn for the first time) myriad aspects of quantum electronics and exciting to be working in a "hot" and controversial area. It has also been rejuvenating for Lewis to be a graduate student in the lab on this project for the time being until funding can be secured. Meanwhile, their long-time friends and colleagues, **DR. RALPH YOUNG** and **DR. AL MARCHETTI**, continue with their own OLED-related research and are close to a new publication from the lab on the physics of charge injection.

Lewis has developed even greater passion for teaching and has exercised it in continuing to develop the General Chemistry course (CHEM 137) for engineers in Fall. The latest innovation for connecting Gen Chem to real sustainability problems is a series of video homeworks supported by Dean Rachel Remmel in the learning center and Jason Wagner in IT, and filmed by a professional firm. The initial set of videos involves connecting the course materials to frontier problems (Chemistry of Greenhouse Gases, Development of Solar Fuels, Redox Flow Batteries for Grid Storage) and then interviewing scientists doing research at the frontier in these areas. With the help of an outstanding senior Chemistry major, **ERIN STOCKDALE**, they interviewed Professor Vas Petrenko (EES) on his atmospheric methane work, Todd Krauss and Kara Bren on their hydrogen photogeneration work using quantum dots and biocatalysts, and Mamta Dagar (Matson group graduate student) on her studies of polyoxovanadate clusters for redox flow battery applications.

Along with a number of faculty, Lewis is spearheading the work to tailor the Open Stax online Atoms First General Chemistry text to be used as a UofR customized free text in future versions of CHEM 131 and 132. As part of that effort, many of the useful and interesting aspects of learning theory as taught in the workshop training program developed by Jack Kampmeier and successors are reviewed for the students in a preface to the new book. The quality of the content in the Open Stax book is excellent, a tribute to the Chemistry community at large who assembled it, and they are proud to have a customized version for the Department's own General Chemistry sequence.

Lewis accepted a role to serve the Department as Associate Chair. The administrative burden for Departmental Chairs has become consuming, and he

hopes to support Kara in at least a few small aspects of her responsibilities. So far, Lewis has enjoyed working with the administrative staff and interfacing with parts of the Dean's office responsible for accreditation and teaching effectiveness.

Shelby remains CTO of Mosaic Microsystems which is growing rapidly in that race for profitability. It is intellectually and managerially challenging work that brings with it the gratification of helping to bring manufacturing jobs to the Rochester community.

Charles will be a senior at the University of Wisconsin at Madison in Political Science and is fast becoming integrated into Wisconsin politics. Vivian is beginning her second year at Brandeis and is interested in a wide variety of pursuits.

Lewis is planning to retire and join the Faculty Senior Associates Program in mid-2024 that will enable him to continue with research, curriculum development and science writing for the public. As he sometimes jokes, "I needed to retire so I could get some work done." He will deeply miss classroom teaching, especially General Chemistry, but plans to continue to develop materials for both University teaching and for the general public that highlight the role of Chemistry in both contributing to and potentially remediating important environmental sustainability challenges.

Flower in bloom on campus

Michael T. Ruggerio

Associate Professor of Chemistry — Ph.D. 2016, Syracuse University

RESEARCH INTERESTS

Physical chemistry: condensed phase vibrational spectroscopy of materials, structure-property-dynamics relationships in organic materials, development and application of solid-state quantum mechanical and artificial intelligence simulation methods.

CONTACT

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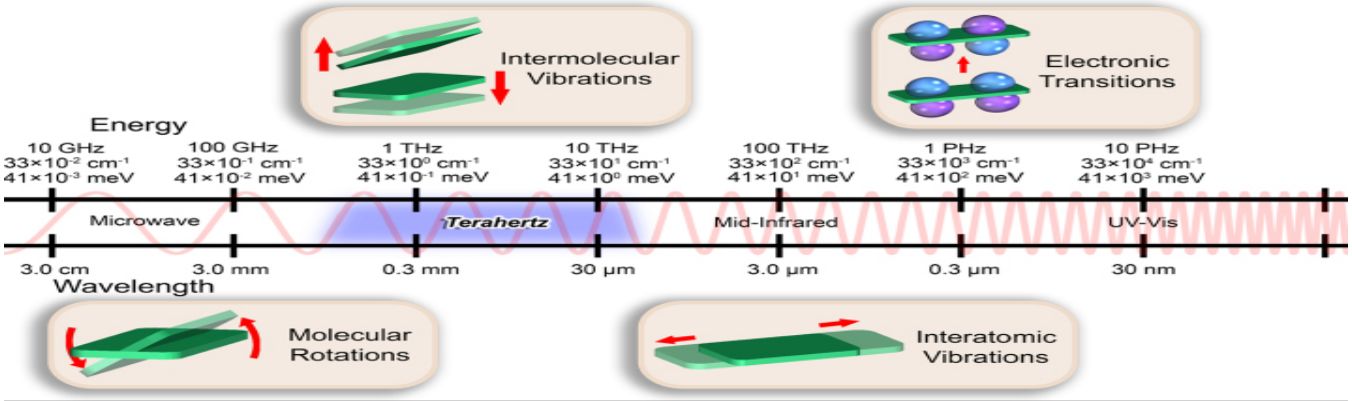
MICHAEL (MIKE) RUGGIERO is a new Associate Professor in the Department of Chemistry, who has joined the University of Rochester after a 5-year stint as faculty member at the University of Vermont. He is a native of Long Island, New York, and a graduate of SUNY Geneseo and Syracuse University, and he is excited to return 'home' to Western New York to continue his career. His research is focused on utilizing low-frequency vibrational spectroscopy (far-infrared or terahertz radiation) to understand the nature of the interactions between molecules in condensed phase materials. This builds on his PhD studies from Syracuse, and his postdoctoral work at the University of Cambridge in the United Kingdom, and is a continuation of his independent work from Vermont. The research interests of the Ruggiero Lab cover a broad class of materials, including solar conversion crystals and photovoltaics, molecular sieves for gas harvesting and storage applications, pharmaceuticals, and understanding strong-field light-matter interactions, to name a few. He is the recipient of a number of awards, including a NSF CAREER award, Forbes 30 under 30, and the Young Scientist Award from the International Society of Infrared, Millimeter, and Terahertz Waves. He is an editor of the ACS journal *Crystal Growth & Design*, and has been named an Emerging Investigator by *Chemical Communications,* the *Journal of Materials Science*, and *Crystal Growth & Design*.

At Rochester, the Ruggiero Group will continue to focus on understanding the low-frequency vibrational response of materials. Low-frequency (terahertz) vibrational spectroscopy (0.3 - 10 THz, 10 – 333 cm-1) has exploded in popularity over the last decade, as advances in technology and applications have resulted in countless significant scientific breakthroughs that have opened multiple new and exciting lines of research. Low-frequency vibrational spectroscopy involves long-range collective motions of entire molecules in the condensed phase, making it a powerful tool for understanding the weak forces that govern endless bulk phenomena. In addition to being a powerful probe of intermolecular interactions, the motions that occur at terahertz frequencies are increasingly being shown to be directly responsible for driving many dynamical processes that are critical to advanced materials. Because terahertz modes involve large-amplitude collective displacements – for example rigid-body hindered translations and rotations, and intramolecular torsions – they map out a large portion of the multidimensional potential energy surface. Over the last few years, these motions have been mapped, directly, to dynamic phenomena such as phase transformations, enzymatic catalysis, mechanical response, and reactivity, amongst others. This has not only led to an unprecedented view into the particular atomic-level mechanisms of these



processes, but also has opened the door to controlling these phenomena using terahertz radiation alone. The goal of this research program is to gain a thorough understanding of how terahertz dynamics dictate material function, and to ultimately utilize this knowledge to gain coherent control over such processes using terahertz radiation alone. This research program spans traditional disciplinary lines, and will involve a broad set of projects that involve not only terahertz method development and application, but also development of new theoretical tools, chemical synthetic protocols, crystal engineering, and electronic device fabrication.

Rochester is an exciting institution at which to perform this transdisciplinary research. Mike and his team will continue to fully-leverage the resources available at the University of Rochester to bring together diverse experts to answer cutting-edge questions related to advanced material design and applications. From the Institute of Optics to the Laser Lab for Energetics, the Ruggiero Group will forge exciting new collaborations across campus in order to bring the joys of terahertz spectroscopy to a new subset of researchers.

Outside of the lab, Mike enjoys spending time with his wife Danielle, 18 month old son, Everest, and his two dogs, Cooper and Julep. You will likely find the Ruggiero's searching for new hiking trails and fun places to walk the dogs, or exploring the booming Rochester local food and craft beer scene. Mike is a huge fan of music and he is excited to start seeing shows at familiar musical venues, including CMAC in Canandaigua, Darien Lake, Lakeview Ampitheatre in Syracuse, and of course – returning to the Carrier Dome in Syracuse for football and basketball games.

Michael Ruggeiro, his wife Danielle, and their child Everest enjoy the great outdoors.

Wolf-Udo Schröder

Professor of Chemistry and Physics Ph.D. 1971, Technical University Darmstadt, Germany

RESEARCH INTERESTS

Basic and applied nuclear science: Dynamics of nuclear reactions at low and medium energies; non-equilibrium transport phenomena; thermodynamics of nuclear disintegration and transmutation. The role of nuclear particle correlations and cluster effects in reactions relevant for nuclear plasma-, fusion-, and astrophysics. Radiation-chemistry experiments on tritium transport in metals, chemi-and physi-sorption.

CONTACT

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W. UDO SCHRÖDER'S Nuclear Science Research Group has continued with two collaborative projects, a radio-chemical study of tritium transport in metals and an experimental nuclear physics program investigating reactions between light nuclei.

The goals of the radio-chemical research are to develop efficient methods to isotopically separate the working fuel gas mixture of DT fusion reactors and to efficiently store the radioactive tritium component generated in situ. Several types of DT fusion reactors are currently under development in the U.S. industry.

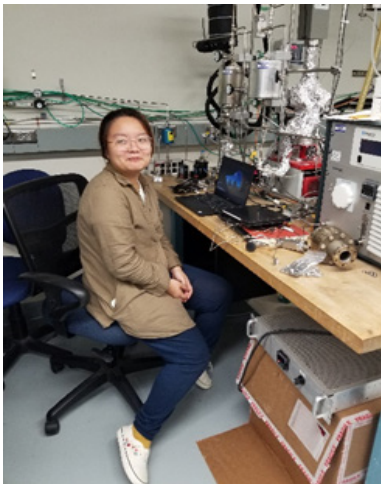
Graduate student **JOSH RUBY** completed a series of variations of the super-permeator setup at the UR Laboratory for Laser Energetics (LLE) shown in the first picture. He has run successful measurements of protium permeation with a thin alpha-iron permeator foil. An extensive scanning of the parameter space is now underway.

Undergraduate student **EVA LIU** is shown in the second picture at an experimental storage test experiment at LLE involving a molecular sieve column. Such a device could prove an efficient and economically attractive isotope separator and storage container of any isotope of hydrogen. As such, the device could see applications on a grand scale in a future "hydrogen economy," where regular hydrogen is used as a transportation fuel or for intermediate storage in non-dispatchable, renewable-energy generation.

As breaking news involving a recent graduate of the group, we are happy to congratulate **CODY FAGAN** on his ascension to CEO of the Rochester Branch of Thorion, a company serving the nuclear fusion energy industry. Congratulations to former graduate of the group, **SHETH NYIBULE**, for his appointment to the UR faculty in Physics and Astronomy.

In the nuclear physics program of the group, the new experimental platform LIANS (Laser Ion Acceleration for Nuclear Science) has been used to produce and improve energetic (MeV) beams of deuterons, as chemically equivalent of the radioactive triton ions. Former graduate student **ARNOLD SCHWEMMLEIN,** now Postdoctoral Researcher in the High Energy Density Physics group, has published the results of the recent experimental runs in Nuclear Instruments and Methods (2022) and has presented the results on several national and international meetings.

Graduate Student Josh Ruby at his Permeation Experiment at the LLE

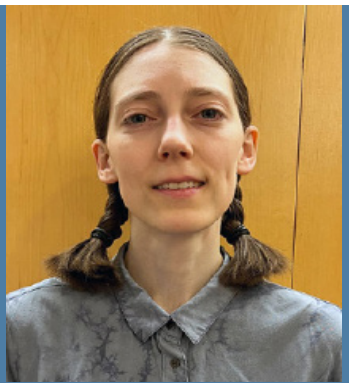


Undergraduate student Eva Liu at her molecular sieve setup at LLE.

Agnes Thorarinsdottir

Assistant Professor of Chemistry

Ph.D. 2020, Northwestern University



RESEARCH INTERESTS

Applies the tools of synthetic molecular and materials chemistry to the design of new electrochemical systems that address challenges in energy, catalysis, and environmental sustainability.

CONTACT

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AGNES THORARINSDOTTIR joined the Department on July 1, 2023, as an assistant professor. She is a native of Iceland and obtained her BS degree in chemistry from the University of Iceland in Reykjavik in 2015. She then moved to Evanston, IL, to pursue her PhD degree in chemistry at Northwestern University with Professor Dave Harris. Her dissertation research centered on employing coordination chemistry approaches to control electronic spins in transition metal compounds in efforts to design bioresponsive magnetic resonance imaging probes and metal–organic magnetic materials. Upon graduation, she relocated to the East Coast and joined the laboratory of Professor Daniel Nocera at Harvard University as a postdoctoral fellow in January 2020. At Harvard, Agnes held a Harvard University Center for the Environment postdoctoral fellowship, and her work focused on addressing challenges in energy science and catalysis through the design of novel electrocatalytic systems. She spearheaded a collaborative effort between the Nocera and Mason groups at Harvard in employing microporous water to achieving supersaturated aqueous solutions of small gas molecules (e.g., O_2, CO_2) that may react at enhanced current densities and under no or minimal mass transport limitations in reactions of energy relevance. She also developed water oxidation catalysts based on earth-abundant elements that may operate in acidic solutions.

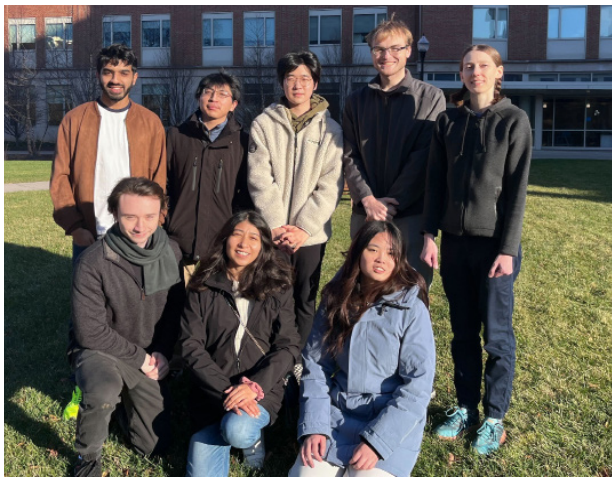
At the University of Rochester, Agnes is super excited about merging her expertise in inorganic and materials chemistry, electrochemistry, and catalysis to create a research program that seeks to apply the tools of synthetic molecular and materials chemistry to the design of new electrochemical systems that address challenges in energy, catalysis, and environmental sustainability. Specifically, the Thorarinsdottir Group is developing new synthetic strategies for enabling precise control of the chemical and physical properties of electrochemical interfaces in efforts to increase the energy efficiency and selectivity of reactions and devices. Particular emphasis is placed on creating new electrochemical systems for:

(i) sustainable production of electricity, fuels, and chemicals,

(ii) efficient energy conversion, and

(iii) electrochemical sensing.

This past summer, Agnes set up her lab in the basement of Hutchison Hall. She was very fortunate to receive tremendous help from two talented undergraduate students, **BRYCE KNEER** ('25) and **DUONG TRUONG**. Bryce is finishing up his junior year at the University and has continued doing research in the Thorarinsdottir Group over the academic year. Duong was part of the iScholar program and has now returned to Singapore, but they hope he will join them again soon! The team has grown a lot since the summer, as three undergraduate students, **JAMES KIM** ('25), **MEIQIN GAO**('24), and **STEVEN RIERA** ('25) joined in September, and three first-year graduate students, **ANYESH DE, DANIELA CARMONA PEREZ** and **PHILLIP DINGA** joined the group at the end of November. All members have now started their individual projects and are looking forward to the summer, when they can devote full effort to their research. They will have two additional undergraduate students (one iScholar and one REU student) with them over the summer and a postdoctoral fellow is also joining in July. There are exciting times ahead!



Commencement 2019

Bachelors and Masters Degrees Awarded in Chemistry

2019 BACHELOR OF SCIENCE

Yifeng Bian
Jieyu He
Garrett Hoteling
Benjamin Lerner
Renee Niles
Aidan Oi
Allison Stanko
Cullen Walsh
Zhihao Wu

2019 BACHELOR OF ARTS

Oswaldo Aguirre
Ian Brodka
Marco Caiola
Lea Domondon
Ryan Fanning
Patrick Forrestel
Ziyu Jia
Andrew Lee
Nicholas Lim
Robert Love
Ryan Newbauer
Megan Ngai
Robert Scappaticci
William Schlageter
Rebecca Sheets
Emmanuel Yanta

2019 MASTER OF SCIENCE

Brittany Abraham
Diego Arevalo
Andrew Bortz
Joshua DeMuth
Steven Diaz
Emily Edwards
Alex Fertig
Maitrayee Ghosh
Yu Gu
Connor Holt
Jacob Iannuzzelli
Melissa Koch
Donggeon (Albert) Nam
Elena Quigley
Mikhalia (Kylie) Ritz
Dominick Sarappa
Bradley Schurr
Jacob Shelton
Trevor Tumiel
David Vargas

Commencement 2020

Bachelors and Masters Degrees Awarded in Chemistry

2020 BACHELOR OF SCIENCE

John Clay
Jessica Conforti
Marissa Coschigano
Brendan Courtsal
Ruilin Gao
Lillian Huntoon
Jana Jelušić
Julian Maceren
Michela Maiola
Philip Palermo
Aneara Ren
Annabel Selino
Paul Sinclair
Jisoo Woo

2020 BACHELOR OF ARTS

Yimin Talia Chen
Ziyu Jia
Aidan Kendra
Samantha Kerber
Chanbin Lee
Cassidy Leight
Chunhao Liu
Tyler Mason
Tanner Metcalfe
Colin Murphy
Zhenhuan Rick Qiu
Jacob Rozowsky
Paulash Sarma
William Schlageter
Gilbert Smolyak
Andrew Sopchak
Logan Worley

2020 MASTER OF SCIENCE

Maria Aguilera
Nikki Bakas
Erin Christensen
David Detloff
Jackson Hernandez
Kaitlyn Houghtling
Melissa Jagrosse
Michael Klaczko
Emily Lasher
Robert Potenzino
Karla Sanchez Lievanos
Eric Schreiber
Prakhar Swarup
Jakub Vaith
Geemi Wellawatte
Francine Yanchik

Commencement 2021

Bachelors and Masters Degrees Awarded in Chemistry

2021 BACHELOR OF SCIENCE

Ahshabibi Ahmed
Timur Cinay
Sarah Craig
Matt DeLorenzo
Justine Drappeau
Dalton Hanaway
Jade Johnson
Noelle Peluso
Alfons Pineda-Knauseder
Jacob Schmidt

2021 BACHELOR OF ARTS

Yi Bu
Joanna Chavez
Clara Hope Simpson
Elaine Kupets
Evelyn Matei
Colin Murphy
Rushika Nama
Caleb Prus
Hannah Roberts
Joshua Rosario
Tayfun Sahin
Paulash Sarma
Yeonseong Seo
Katherine Stankevich
Zhiwei Wang

2021 MASTER OF SCIENCE

Vijay Mocherla
Suchen Wan
Ryan Ballirano
John Bennett
Shilpa Bhatia
Amanda Canfield
Ethan DeCicco
Hannah Distaffen
William Girten
Kathryn Goerl
Christopher Jones
Anees Keedakkatt Puthenpeedikakkal
Aleksa Milosavljevic
Darya Rodina
Alison Salamatian
Abhijith Saseendran
Anitha
James Stair
Vishal Tiwari

Commencement 2022

Bachelors and Masters Degrees Awarded in Chemistry

2022 BACHELOR OF SCIENCE

Yahia Ali
Daniel Carstairs
Lauren Lopez
Kaelyn McFarlan-Connelly
Yueheng Min
Ryan Pohorenec
Elliot Silk

2022 BACHELOR OF ARTS

Anca Frasineanu
Jenna Jeffway
Gloria Kim
Eleanor Mancusi-Ungaro
Madalayne Martin-Olenski
Collin Murphy
Isabella Orup
Den Khi Son
Katherine Stankevich

2022 MASTER OF SCIENCE

Ronald Adukure
Medina Afandiyeva
Nathalia Cajiao
Ignacio Camarero Temino
Chayan Carmenate Rodriguez
Rachel Garwick
Magali Gimeno
Ignacio Gustin
Dalton Hanaway
Christopher Hastings
Eric Koessler
Ryan Kosko
Kaye Kuphal
Alexa LaPierre
Robert Lewis
Kacie Malyk
Caitlyn McNichol
Aurodeep Panda
Joshua Ruby
Mary Siriboe
Bevan Whithead
Wenxiang Ying

Commencement 2023

Bachelors and Masters Degrees Awarded in Chemistry

2023 BACHELOR OF SCIENCE

Erika Cerna Arroyo
Elise Gendrich
Yahui (Leyla) Guo
Maxwell Hughes
Aidan Kropiwnicki
Yitian Liu
Daniel T. Nakamura
Rylee Stuart Neumann
Aliza Panjwani
Camden Reid Parker
Jacob Ritterman
Tong Sun
Jialong Wang
Xijue Wu
Xiaotian Zhang
Zeyuan Zhu

2023 BACHELOR OF ARTS

Seungjae Chun
Emily Diaz
Ciara Fernandez
Ellen Irving
Thompson V. Marinho
Lily Neugebauer
Erin O'Kane
Camille E. Stevenson
Hannah Shanley
Luci Vosatka
Griffin C. Weiner
Jiwon Woo
Ahjin Yoo

2023 MASTER OF SCIENCE

Pamela Agredo
Daniel Akuamoah
Farwa Awan
Alexis Bauer
Roberto Leon Baxin
Jordan Butt
Shannon Cooney
Bo Couture
Erica Craddock
Mamta Dagar
Thakshila Dayananda
Michelle Hendricks
Hafsa Irfan
Nawal Jafari
Maria Lizarazo
Yeuheng (Sam) Min
Hailemariam Mitiku
Owen Monteferrante
Sebastian Montillo
Soraya Ngarnim
Shannon, O'Neil
Chari Peter
Liz Phinney
Liz Piedmont
Vivek Gangadharan Pillai
Ryan Pohorenec
Katie Proe
Revathy Rajan
Leyla Valerio
Juan Villada Morales
Patrycia Zybura

Doctoral Degrees Awarded in Chemistry

2019

Hanan Alwaseem
Late-stage Functionalization of Sesquiterpenoids via Engineered P450 Enzymes
Advisor: Rudi Fasan

Tessa Baker
Insights into Iron Chemistry in Nature and Catalysis through Electronic Structure, Bonding, and Mechanism Studies
Advisor: Michael Neidig

Valerie Fleischauer
Applications of Physical Inorganic Spectroscopy to d – and f – block Metals: Catalysis, Electronic Structure, and Bonding
Advisor: Michael L. Neidig

Abigail Freyer
Investigation of Doped Nanocrystals Utilizing electrostatic force microscopy
Advisor: Kara Bren

Yixing Guo
Cobalt Metallopeptide for Multi Proton, Multi Electron Reactions
Advisor: Kara Bren

Patrick Harrington
I. Studies Towards an Iodoaldol Addition and cationic Cyclization Reaction
II. The 1,6 Conjugate Initiated Nazarov and 1,5 transfer Initiated Cascade Cyclization
Advisor: Alison Frontier

Andrew Kauffmann
Structures of RNA sequences from influenza A virus
Advisor: Douglas H. Turner

Michael Mark
"Excited State Dynamics of Organic Chromophores Used in Solar Hydrogen Production"
Advisor: David McCamant

Andrew Owens
Strategies for the Evolution of macrocyclic Peptide Inhibitors of Protein-Protein Interactions
Advisor: Rudi Fasan

Danielle Riegle
Multicomponent Supramolecular Peptide Biomaterials
Advisor: Bradley L. Nilsson

Kyle William Rugg
I. Second-Generation Total Synthesis of (-)-Nakadomarin A
II. Studies Toward the Total Synthesis of (-)-Apoptolidin A
Advisor: Robert Boeckman, Jr.

Eric Stoutenberg
Studies toward the Total Synthesis of Tetrapetalone A
Advisor: Alison Frontier

Jing Yuwen
Activation of O-H/N-H bonds by Rhodium Complex
Advisor: William Jones

2020

Rebeckah Johnson Burke
Colloidal Semiconductor Nanocrystals for Photocatalytic Proton Reduction
Advisor: Todd Krauss

Stephanie Hope Carpenter
Intermediates in Base Metal Catalysis for Organic Transformations: Cross-Coupling and C-H Functionalization
Advisor: Michael L. Neidig

Saikat Chakraborty
Development of Photocatalytic Systems for Hydrogen Production from Water
Advisor: Kara Bren

Theresa Elizabeth Iannuzzi-Boddie
Structure and Mechanism in Iron-and Cobalt-Catalyzed Directed C-H Functionalization
Advisor: Michael L. Neidig

Zhi Li
Frontiers in the Atomistic Modeling of Molecular Junctions: Bringing Theory Closer to Experiment
Advisor: Ignacio Franco

John D. McAnany
Novel Approaches to RNA-Targeted Compound Discovery; Searching for TeV Gamma-ray Emission from Compact Binaries with the HAWC Observatory
Advisor: Benjamin L. Miller

Justin M. Niziol
Part I. A Scalable Synthesis of (-)-Rasfonin Enabled by a Convergent Enantioselective α-Hydroxymethylation Strategy. Part II. Studies Towards the Total Synthesis of FK-506
Advisor: Robert Boeckman Jr

Astrid Marisol Parsons
I. Transition-Metal-Catalyzed Reactions: Harnessing Metals to Facilitate Organic Transformation
II. Statistical Methods for Treatment Evaluation with Application to Longitudinal Studies
Advisor: William D. Jones

Dylan E. Parsons
I. Cationic Cascade Reactions of Alkylidene β-Ketoesters
II. Studies Toward the Total Synthesis of Arnicenone
Advisor: Alison Frontier

Zachary Tyler Piontkowski
Excited State Torsions and Electron Transfer in Dye Sensitizers for Light Harvesting and Photodynamic Therapy
Advisor: David McCamant

Viktoria Charlotte Steck
Biocatalytic Methods for Carbon-Nitrogen Bond Formation via Hemoprotein-Catalyzed Group Transfer Reactions
Advisor: Rudi Fasan

Sreyoshi Sur
Membrane Selectivity of Fengycin, an Antimicrobial Lipopeptide using Molecular Simulations
Advisor: Alan Grossfield

Oliver L. R. Swart
Analysis and Effect of Small-Molecules Targeting Pre-MicroRNA Structures and Synthetic Efforts Toward a Novel Scaffold for RNA Targeting
Advisor: Benjamin L. Miller

Jennifer M. Urban
Super-Resolution Biological Imaging with Quantum Dots
Advisor: Bradley Nilsson and Todd D. Krauss

Lauren Elizabeth VanGelder
Polyoxovanadium-Alkoxide Clusters as Charge Carriers for Nonaqueous Redox Flow Batteries
Advisor: Ellen Matson

Jade J. Welch
Disulfide Constrained Peptides: Properties and Application
Advisor: Bradley Nilsson

2021

Georgios Alachouzos
Development of the Interrupted halo-Nazarov Reaction Methodology, Computational and Natural Product Synthesis Studies Towards Complex Halcyclopentenes
Advisor: Alison Frontier

Sutirtha Narayan Chowdhury
Incorporating nuclear quantum effects for investigating non-adiabatic dynamics
Advisor: Pengfei Huo

Tarah DiBenedetto
Transition Metals in Catalysis: Harnessing Metals to Form Carbon-Carbon and Carbon- Boron Bonds
Advisor: William D. Jones

Phuong Hang (Jennifer) Le
Catalytic Hydrogen Evolution by a Synthetic Cobalt Mini-enzyme
Advisor: Kara Bren

Joohyun Lee
Ultrafast Dynamics of Photoexcited DNA Nucleotides Probed with Femtosecond Stimulated Raman Spectroscopy
Advisor: David McCamant

Eric Moore
Design of Artificial and Thermostable Myoglobin-based Biocatalysts for Carbene Transfer Reactions
Advisor: Rudi Fasan

Brittney Petel
Synthesis, Characterization, and Reactivity of Oxygen-Deficient Polyoxovanadate-Alkoxide Clusters
Advisor: Ellen Matson

Antonio Jose Garzon Ramirez
Ultrafast control of electrons using few-cycle laser pulses
Advisor: Ignacio Franco

Julie Smyder
Elucidating the Single-Molecule Fluorescence Intermittency and Quantum Yield of Nanoscale Particles with Confocal and Scanning Probe Microscopies
Advisor: Todd Krauss

Antonio Tinoco Valencia
Biocatalytic Organofluorine Synthesis via Hemoprotein-Catalyzed Carbene Transfer Reactions
Advisor: Rudi Fasan

Jianbo Zhao
Molecular Dynamics and Quantum Mechanics Studies of RNA Structures
Advisor: Douglas Turner

2022

Jose Luis Alvarez-Hernandez
Bioinspired Cobalt Catalysts for Electrochemical Hydrogen Evolution and CO2 Reduction in Water
Advisor: Kara Bren

David A. Brewster
Synthesis and Electrochemical Characterization of Metal Oxide Nanocrystals as Model Systems for Battery Electrodes
Advisor: Kathryn Knowles

Nicole M.B. Cogan
Photophysical Properties of (I) Single-Walled Carbon Nanotubes and (II)an Unknown Single-Photon Emitter
Advisor: Todd D. Krauss

Cody E. Fagan
Tritium Interactions with Stainless Steel Type 316
Advisor: Wolf-Udo Schroeder

Xinyang Li
Controlling Chemical Reactivities Beyond Existing Paradigms
Advisor: Pengfei Huo

Ningyu Liu
Biocatalytic Methods for Carbene Transfer Reactions
Advisor: Rudi Fasan

Arkajit Mandal
Quantum Dynamics Simulation of Photons and Molecules
Advisor: Pengfei Huo

Analuz Mark
Chapter 1. Direct Experimental Evidence of Alkoxyl Radicals Reacting as Hydrogen Atom Donors Towards Pyridines Chapter 2. Novel Emissive Intramolecular Organic Cationic Exciplexes in Water
Advisor: Joseph P. Dinnocenzo

Leopoldo Mejia Restropo
Mechanical Control of Charge Transport and Chemical Reactivity in Molecular Junctions
Advisor: Ignacio Franco

Rachel Linette Meyer
The Electronic Structure and Reactivity of Heterometal-Functionalized Polyoxovanadate Clusters
Advisor: Ellen Matson

Jeffrey D. Sears
Adventures in Metal-Hydrocarbyl Chemistry: Iron-Catalyzed Carbon-Carbon (C-C) Cross-Coupling Mechanism and Fundamental Homoleptic Organouranium Chemistry
Advisor: Michael L. Neidig

Jesse Raymond Stroka
Electrocatalytic Nitrate and Nitrite Reduction by Inorganic Complexes
Advisor: Kara L. Bren

Mehrin Blinth E. Tariq
Investigation of Surface Chemistry and Catalytic Properties of Colloidal Cu_2O Nanoparticles
Advisor: Kathryn Knowles

Andrew I. VanderWeide
Mechanistic Studies on C-H Activation and Development of FOX Complexes
Advisor: William D. Jones

David Vargas
Biocatalytic Strategies for the Synthesis and Functionalization of Heterocycles via Abiotic Myoglobin-Catalyzed Reactions
Advisor: Rudi Fasan

Liwei Wang
Understanding the Correlation between Microscopic Morphology and Photophysical Properties of Conjugated Polymers by Optical Spectroscopy
Advisor: Lewis Rothberg

Nikki Jo Wolford
Synthesis and Electronic Structure in Iron and Uranium Coordination Complexes
Advisor: Michael L. Neidig

2023

Brittany Abraham
Development of Low Molecular Weight Phenylalanine-Derived Supramolecular Hydrogels
Advisor: Bradley L. Nilsson

Maria Camila Aguilera
Intermediates, Reactivity and Mechanisms in Iron-Catalyzed Cross-Coupling Reactions Supported by Bisphosphine Ligands
Advisor: Michael L. Neidig

Nikki Joanna Bakkas
Additive and Ligand Effects in Iron-Catalyzed C-C Bond Forming Reactions
Advisor: Michael L. Neidig

Shilpa Bhatia
Elucidating Intermediates and Mechanism in Iron-Catalyzed C-H Activation/Functionalization Reactions
Advisor: Michael L. Neidig

Andrew Bortz
Late Stage Chemoenzymatic Diversification of Natural Products and Bioactive Molecules
Advisor: Rudi Fasan

Joshua Collin DeMuth
Mechanistic Elucidation in Iron-Catalyzed C-H Activation/ Functionalization
Advisor: Michael L. Neidig

Emily Edwards
Developing Bioinspired Systems for Photocatalytic Evolution
Advisor: Kara L. Bren

Alex Fertig
Modeling the Reactivity of Proton Coupled Electron Transfer at the Surface of Heterogeneous Metal Oxide Materials through the use of Polyoxometalate Clusters
Advisor: Ellen Matson

Yu Gu
Design and Development of Macrocyclic Peptide Agents and MacrocycleAntibody Fusions for Targeting Protein Interfaces
Advisor: Rudi Fasan

Jackson J. Hernandez
Developing Methods for Aza/Oxa- Alkynyl Prins Cascades and Nazarov-Type Cyclizations
Advisor: Alison J. Frontier

Connor Holt
Developing the halo-Prins/halo-Nazarov: Disrupting Aromaticity, Chirality Transfer, and Studies toward Natural Product Synthesis
Advisor: Alison J. Frontier

Jacob Iannuzzelli
Leveraging genetic code expansion for cyclopeptide discovery and protein stabilization
Advisor: Rudi Fasan

Melissa Jagrosse
Novel Biomaterials for the Functional Delivery of Biological Macromolecules
Advisor: Bradley L. Nilsson

Michael E. Klaczko
Applications of Microporous Nanomembranes for the Detection and Study of Infectious Diseases
Advisor: James McGrath

Melissa Koch
Electrochemistry of Transition Metal Oxide Nanomaterials and their Photoelectrocatalytic Performance
Advisor: Kathryn Knowles

Donggeon (Albert) Nam
Expansion and Elucidation of Biocatalytic Methods for Asymmetric Synthesis with Challenging Carbene Precursors
Advisor: Rudi Fasan

2023

Mikhaila (Kylie) Ritz

The Development of Novel Transition Metal Catalysts and Electrochemical Methods for the Formation of New Carbon-Carbon and Carbon-Heteroatom Bonds

Advisor: William D. Jones

Karla R. Sanchez Lievanos

Exploring the synthesis, surface chemistry and catalytic activity of phase-pure spinel ferrite nanocrystals

Advisor: Kathryn Knowles

Juan Sandoval Cabezas

Theoretical, Computational, and Experimental Modeling of Molecular Excited States

Advisor: David McCamant

Eric Schreiber

Cation-coupled electron transfer to polyoxovanadate-alkoxide clusters : Atomically precise descriptors for energy storage and conversion processes

Advisor: Ellen Matson

Trevor M. Tumiel

Photophysical properties of perturbed single-walled carbon nanotubes

Advisor: Todd D. Krauss

Gemmi Piyatha Wellawatte

Applications of artificial intelligence in chemistry

Advisor: Andrew White

Francine Elizabeth Yanchik-Slade

I. Impact of Solvent Conditions on Pleated and Rippled Beta-Sheet Assembly

II. Development of a Platelet Activation Model in Ischemic Stroke

Advisor: Bradley L. Nilsson

Bufan Zhang

An Account of Iron-Amide Chemistry: Catalysis, Structures, and Spectroscopy

Advisor: Michael L. Neidig

Selected Publications
January 2019 - December 2023

BRANDON BARNETT

Whitehead, B.S.; Brennessel, W.W.; Michtavy, S.S.; Silva, H.A.; Kim, J.; Milner, P.J.; Porosoff, M.D.; Barnett, B.R. "Selective Adsorption of Fluorinated Super Greenhouse Gases within a Metal–Organic Framework with Dynamic Corrugated Ultramicropores." *Chemical Science* **2024**, 15, 5964–5972.

Hastings, C.D.; Huffman, L.S.X.; Tiwari, C.K.; Betancourth, J.G.; Brennessel, W.W.; Barnett, B.R. "Coordinatively Unsaturated Metallates of Cobalt(II), Nickel(II), and Zinc(II) Guarded by a Rigid and Narrow Void." *Inorganic Chemistry* **2023**, 62, 11920-11931.

Barnett, B.R.; Evans, H.A.; Su, G. M.; Jiang, H.Z.H.; Chakraborty, R.; Banyeretse, D.; Hartman, T.J.; Martinez, M.B.; Trump. B.A.; Tarver, J.D.; Dods, M.N.; Funke, L.M.; Börgel, J.; Reimer, J.A.; Drisdell, W.S.; Hurst, K.E.; Gennett, T.; FitzGerald, S.A.; Brown, C.M.; Head-Gordon, M.; Long, J.R. "Observation of an Intermediate to H2 Binding in a Metal–Organic Framework." *J. Am. Chem. Soc.* **2021**, 143, 14884-14994.

KARA BREN

Edwards, E.H.; Jelušić, J.; Kosko, R.M.; McClellend, K.P.; Ngarnim, S.S.; Chiang, W.; Lampa-Pastirk, S.; Krauss, T.D.; Bren, K.L. "Shewanella oneidensis MR-1 Respires CdSe Quantum Dots for Photocatalytic Hydrogen Evolution." *Proc. Natl. Acad. Sci. USA*, **2023**, 120, e2206975120. DOI: 10.1073/pnas.2206975120

Salamatian, A.A.; Bren, K.L."Bioinspired and Biomolecular Catalysts for Energy-Relevant Reactions." *FEBS Lett.*, **2023**, 597, 174-190. DOI: 10.1002/1873-3468.14533. Invited Contribution for Special Issue on "Visions of Bio-Inorganic Chemistry: Metals and Molecules of Life."

Alvarez-Hernandez, J.L; Salamatian, A.A.; Han, J.W; and Bren, K.L. "Potential- and Buffer-Dependent Selectivity for the Conversion of CO2 to CO by a Cobalt Porphyrin-Peptide Electrocatalyst in Water." *ACS Catal.*, **2022**, 12, 14689-14697. DOI: 10.1021/acscatal.2c03297

Alvarez-Hernandez, Han, J.W.; Sopchak, A.E.; Guo, Y.; Bren, K.L."Linear Free Energy Relationships in Hydrogen Evolution Catalysis by a Cobalt Tripeptide in Water." *ACS Energy Lett.,* **2021**, 6, 2256-2261. DOI: 10.1021/acsenergylett.1c00680

Stroka, J.R.; Kandemir, B; Matson, E.M.; Bren, K.L."Electrocatalytic Multielectron Nitrite Reduction in Water by an Iron Complex."*ACS Catal.,* **2020**, 10, 13968–13972. DOI: 10.1021/acscatal.0c03600

JOSEPH DINNOCENZO

Dinnocenzo, J. P.; Mark, A.; Farid, S. "Emissive Organic Exciplexes in Water." *J. Org. Chem.*, **2019**, 84, 7840−7850. DOI: 10.1021/acs.joc.9b00718.

Dinnocenzo, J. P.; Tingson, J.; Young, R. H.; Farid, S. "Solvent Dependence of Cationic-Exciplex Emission: Limitation of Solvent Polarity Functions and the Role of Hydrogen Bonding." *J. Phys. Chem.* A **2020**, 124, 3730–3737. DOI: 10.1021/acs.jpca.0b01774.

Feinberg, E. C.; Dinnocenzo, J. P. "Mechanism and Selectivity of Aryltrimethylgermane Cation Radical Fragmenations." *J. Org. Chem.* **2020**, 85, 8639−8644. DOI: 10.1021/acs.joc.0c01032.

Mark, A.; Feinberg, E. C.; Dinnocenzo, J. P. "Direct Experimental Evidence for Alkoxyl Radicals Reacting as Hydrogen Atom Donors Toward Pyridines." *J. Org. Chem.* **2021**, 86, 7508−7514. DOI: 10.1021/acs.joc.1c00504.

Dinnocenzo, J. P.; Farid, S."Cationic Exciplexes: Role of Hydrogen Bonding in Deactivation and Electronic Coupling." D *ChemPhyChem* **2021**, 22, 1738–1744. DOI: 10.1002/cphc.202100293.

IGNACIO FRANCO

I. Gustin, C.W. Kim, D.W. McCamant, and I. Franco. "Mapping Electronic Decoherence Pathways in Molecules." *PNAS*. **2023**, 120, e2309987120.

L. Mejía, P. Cossio, and I. Franco. "Microscopic Theory, Analysis, and Interpretation of Conductance Histograms in Molecular Junctions." *Nature Comm*. **2023**, 14, 7646.

V. Tiwari, B. Gu, and I. Franco. "Floquet theory and computational method for the optical absorption of laser-dressed solids." *Phys. Rev. B*, **2023**, 108, 064308.

C. W. Kim, J. M. Nichol, A. N. Jordan and I. Franco. "Analog Quantum Simulation of the Dynamics of Open Quantum Systems with Quantum Dots and Microelectronic Circuits." *PRX Quantum 3*, **2022**, 040308.

T. Boolakee, C. Heide, A. Garzón-Ramírez, H. B. Weber, I. Franco and P. Hommelhoff. "Light-field control of real and virtual charge carriers." *Nature,* **2022**, 605, 251-255

ALISON FRONTIER

Frontier, Alison J. "The Not Voodoo website after twenty dynamic years" Invited Comment: *Nature Reviews Chemistry* **2024** DOI: 10.1038/s41570-024-00644-9

Milosavljevic, A.; Holt, C.; Frontier, A. J. "Nitrogen-interrupted Prins-Nazarov fragment coupling cascade for the synthesis of indolines." *Chem. Sci.* **2023**, 14, 5431-5437. DOI: 10.1039/d3sc00986f

Hernandez, J.; Frontier, A. J. "Alkynyl Prins carbocyclization cascades for the synthesis of linear-fused heterocyclic ring systems" *Chem. Sci.*, **2022**, 13, 13836 – 13842 DOI: 10.1039/D2SC04750K

Frontier, A. J.; Sinclair, P. P. "Merging Strategy, Improvisation, and Conversation to Solve Problems in Target Synthesis" *Acc. Chem. Res.* **2021**, 54, 1817-1829 doi: 10.1021/acs.accounts.0c00804

Frontier, A. J.; Hernandez, J. "New Twists in Nazarov Cyclization Chemistry." *Acc. Chem. Res.* **2020** 53, 1822–1832. doi: 10.1021/acs.accounts.0c00284

PENGFEI HUO

Ying, W.; Huo, P. "Resonance theory and quantum dynamics simulations of vibrational polariton chemistry." *J. Chem. Phys.* 28 August **2023**; 159 (8): 084104.

Hu, D.; Huo, P. "Ab Initio Molecular Cavity Quantum Electrodynamics Simulations Using Machine Learning Models." *Journal of Chemical Theory and Computation* **2023** 19 (8), 2353-2368. DOI: 10.1021/acs.jctc.3c00137

Zhou, W.; Mandal, A.; Huo, P. "Quasi-Diabatic Scheme for Nonadiabatic On-the-Fly Simulations." *The Journal of Physical Chemistry Letters* **2019** 10 (22), 7062-7070. DOI: 10.1021/acs.jpclett.9b02747

Bossion, D.; Chowdhury, S.N.; Huo, P."Non-adiabatic ring polymer molecular dynamics in the phase space of the SU(N) Lie group." *J. Chem. Phys.* 28 January **2023**; 158 (4): 044123. https://doi.org/10.1063/5.0133970

Taylor, M.A.D.; Mandal, A.; Zhou, W.; Huo, P. "Resolution of Gauge Ambiguities in Molecular Cavity Quantum Electrodynamics." *Phys. Rev. Lett.* 125, 123602 – Published 17 September **2020**

WILLIAM JONES

Jones, W. "Carbon Capture and Conversion." *J. Am. Chem. Soc.* **2020**, 142, 4955-4957. (DOE) DOI: 10.1021/jacs.0c02356

Nachtigall, O; VanderWeide, A.I.; Brennessel, W.W; Jones, W. "Iron-Based Dehydration Catalyst for Selective Formation of Styrene." *ACS Catal.* **2021**, 11, 10885-10891. (DOE) Editor's Choice doi: 10.1021/acscatal.1c03037

Görlich, T; Frost, D.S; Boback, N; Coles, N. T; Dittrich, B; Müller, P; Jones, W; Müller, C. "Photochemical C(sp)-C(sp2) Bond Activation in Phosphaalkynes: a New Route to Reactive Terminal Cyaphido Complexes LnM-C°P." *J. Am. Chem. Soc.* **2021**, 143, 19365-19373. (DOE) doi: 10.1021/jacs.1c07370

Jones, W. "Selectivity in the Activation of C–H Bonds by Rhodium and Iridium Complexes." *Adv. Orgmet. Chem.* **2022**, 78, 1-34. (DOE) DOI: 10.1016/bs.adomc.2022.03.001

Sébastien Lachaize, Dominique C. Gallegos, Juliana J. Antonio, Abdurrahman C. Atesin, Tülay A. Ateşin and William D. Jones, "Ortho-Fluoro Effect on the C—C Bond Activation of Benzonitrile Using Zerovalent Nickel." *Organometallics* **2023**, 42, 2134-2147. (DOE) DOI: 10.1021/acs.organomet.3c00275

ROSE KENNEDY

Afandiyeva, M.; Wu, X.; Brennessel, W. W.; Kadam, A. A.; Kennedy, C. R. "Secondary-Sphere Preorganization Enables Nickel-Catalyzed Nitrile Hydroboration." *Chem. Commun.* **2023**, 59, 13450-13453. DOI: 10.1039/D3CC04229D (Invited submission to the 2023 Emerging Investigators Collection)

Malyk, K. R.; Pillai, V. G.; Brennessel, W. W.; Leon Baxin, R.; Silk, E. S.; Nakamura, D. T.; Kennedy, C. R. "Distinguishing Competing Mechanistic Manifolds for C(acyl)–N Functionalization by a Ni/N-Heterocyclic Carbene Catalyst System." *JACS* Au. **2023**, 3, 2451–2457. DOI: 10.1021/jacsau.3c00283

Hanaway, D. H.; Kennedy, C. R. "An Automated Variable Electric-Field DFT Application for Evaluation of Optimally Oriented Electric Fields on Chemical Reactivity. "*J. Org. Chem.* **2023**, 88, 106–115, DOI: 10.1021/acs.joc.2c01893

Afandiyeva, M.; Kadam, A. A.; Wu, X.; Brennessel, W. W.; Kennedy, C. R. "Synthesis, Structure, and Hydroboration Reactivity of Anionic Nickel(0) Complexes Supported by Bidentate NHC-Pyridone Ligands." *Organometallics*, **2022**, 21, 3014–3023. DOI: 10.1021/acs.organomet.2c00439 (Selected as ACS Editors' Choice.)

KATHRYN KNOWLES

Beidelman, B. A.; Zhang, X.; Matson, E. M.; Knowles, K. E. "Acidity of Carboxylic Acid Ligands Influences the Formation of VO2(A) and VO2(B) Nanocrystals under Solvothermal Conditions." *ACS Nanosci.* Au, **2023**, 3, 381-388.

Shelton, J. L.; Knowles, K. E. "Polaronic Optical Transitions in Hematite (a-Fe2O3) Revealed by First-Principles Electron-Phonon Coupling." *J. Chem. Phys.,* **2022**, 157, 174703.

Beidelman, B. A.; Zhang, X.; Sanchez-Lievanos, K. R.; Selino, A. V.; Matson, E. M.; Knowles, K. E. "Influence of Water Concentration on the Solvothermal Synthesis of VO2(B) Nanocrystals," *CrystEngComm*, **2022**, 24, 6009-6017.

Sanchez-Lievanos, K. R.; Knowles, K. E. "Controlling Cation Distribution and Morphology in Colloidal Zinc Ferrite Nanocrystals." *Chem. Mater.,* **2022**, 34, 7446-7459.*
*Awarded Honorable Mention for Chemistry of Materials Best Paper Award and highlighted in the associated editorial: Skrabalak, S. E. Chem. Mater., 2023, 35, 9447.

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TODD KRAUSS

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