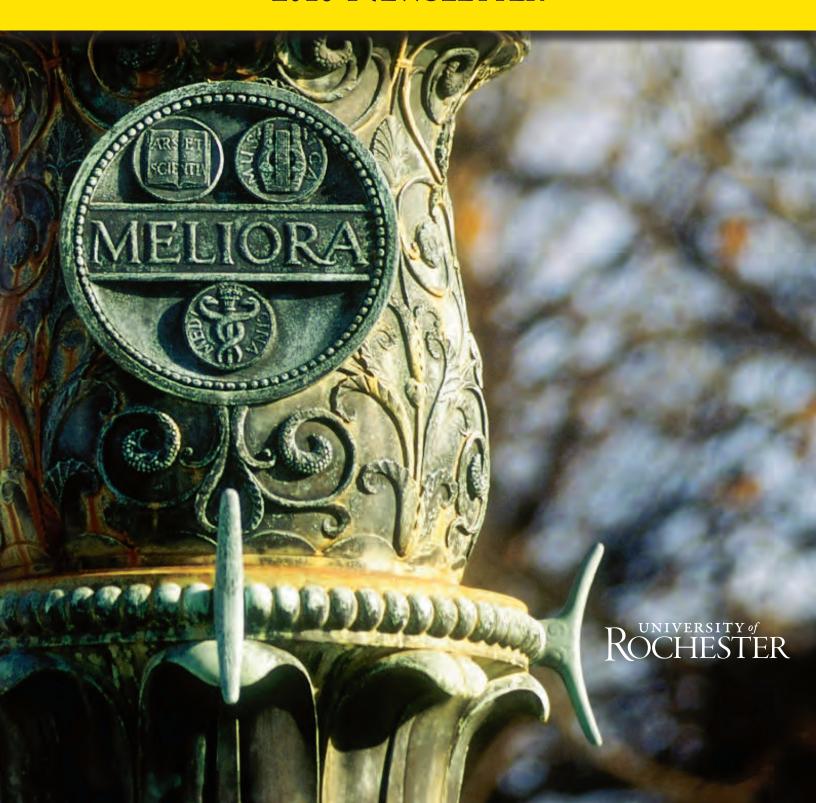
CHEMISTRY

2018 Newsletter





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From the Chair

Greetings to Chemistry Department students, faculty, staff and especially our alumni! I am writing to pass along some of the developments within Chemistry and the University during this past year, my sixth as Chair of the Department.

In sad news, in 2018 the Chemistry Department lost one of its esteemed faculty, as Professor Emeritus Andrew Kende passed away suddenly last February. As those who knew him can attest, Andy had the reputation for demanding excellence in



all facets of his professional career and would not settle for less than the pursuit of science at the highest level in his laboratory. Andy's creativity and vast knowledge of organic chemistry served to inspire his colleagues, and all told he mentored over 50 postdocs and 50 students during his career. Andrew Kende will be missed by not only us here at Rochester, but also the greater chemistry community worldwide.

The Chemistry faculty experienced significant turnover in 2018, as Jim Farrar, Josh Goodman, and Tom Krugh all officially retired from active teaching effective July 2018. First, I want to thank Tom, Jim and Josh for their many years of service to the Department. Collectively they taught over 20,000 undergraduate students during their careers, and for most of my time at Rochester took on some of our most difficult and challenging teaching assignments. Congratulations Jim, Josh and Tom and enjoy your retirements!

The Chemistry faculty continue to be recognized for their excellence in teaching, research and scholarship. In particular, we want to highlight the accomplishments of several faculty including Kara Bren who was selected as an AAAS Fellow, Pengfei Huo who won the National Science Foundation CAREER Award, and Katie Knowles who was a recipient of a University Furth Fund Award. Also, early in 2018 Bill Jones won a prestigious Humboldt Research Award to spend time doing research in Germany. Ellen Matson had a banner year: she won the 2018 Edith Flanigen Award, was one of five inaugural recipients of the Course Hero Woodrow Wilson Fellowship for Excellence in Teaching, and was selected as a Scialog Fellow by the Research Corporation for Science Advancement. Congratulations to Dave McCamant for being selected as the first recipient of The College Award for Undergraduate Teaching and Research Mentorship.

As is no surprise to anyone reading this Newsletter, at Rochester we have the pleasure of teaching, mentoring, and working in the laboratory with some exceptionally talented undergraduates dedicated to learning chemical sciences. While we have by all accounts a tremendously rigorous curriculum, we are always looking to improve the educational outcomes of our students as we adapt to the changing nature of Chemistry. One initiative that was started this year with respect to improving the undergraduate educational experience concerns CHM 232 and 234 our advanced synthetic laboratory techniques and molecular spectroscopy laboratory courses, respectively. Prof. Ellen Matson and Prof. Katie Knowles plan to develop a series of new experiments for these classes in order to integrate experiential, project-based learning into an upper level laboratory course. The new laboratory modules will give students experience with real problem-based research that will prepare them to conduct formal independent research projects with Chemistry faculty.

In May of 2018 we graduated 29 seniors, who will pursue a variety of interests ranging from working at companies around the country, obtaining advanced degrees in biomedicine, chemistry and related STEM fields, attending law school, volunteering, to teaching the next generation of high school chemists. Also, some graduates who can't get enough of Rochester plan to stay on campus for a 5th year taking advantage of either our Take 5 or Master's Degree programs. Going forward we will have close to 50 Chemistry majors in the senior and junior classes this coming academic year, which is about our historical average. Note that if you want to see what our B.A., B.S., M.S. and Ph.D. graduates from 2018 are up to, please check out the exciting new webpage from the Career Center: https://www.rochester.edu/careercenter/about/outcomes/index.html.

The research accomplishments of our graduate students and postdoctoral associates are what drives and underpins the reputation of the University of Rochester as a premier place to pursue advanced chemistry studies. I hope you

will read about all their exciting discoveries in this newsletter! I have a couple of special mentions to pass along, although by no means is this a complete list. I want to congratulate Lauren VanGelder who won our recently endowed Outstanding Graduate Student Award. Students who won prestigious travel awards from the American Chemical Society in 2018 include Brittney Petel, Viktoria Steck, and Antonio Tinoco Valencia. Postdoctoral scholars Farnaz A. Shakib and Bing Gu also won awards in 2018 for their work and were invited to present talks at the American Chemical Society National meeting on their accomplishments. Finally, Antonio Tinoco Valencia and Arkajit Mandal also won awards for their presentations at internationally attended conferences in 2018.

One of my goals for the Department for the near future is to rapidly bring the Department back to our allotted strength with respect to tenure track faculty size. To that end, I am very excited to report that last year we received permission to hire six tenure track faculty over the next three years! Given the renovations needed in Hutchison Hall when hiring new faculty to bring laboratories up to modern standards, the hiring of 6 new faculty represents an investment in Chemistry by the administration of over 15 million dollars. Last year we were thrilled to be able to recruit to Rochester Shauna Paradine, the first of these new hires, who arrived on campus last July. Shauna is an organic chemist who is interested in leveraging the tools of reaction discovery, transition metal catalysis, and mechanistic investigation to solve important problems in organic synthesis. Currently we have an ongoing search for an organic and an inorganic chemist, and I hope to be able to share the outcomes of those searches next year! These hires will allow us to eventually expand faculty size to 26 (from the current 20) over the next roughly 7-10 year timeframe.

Endowed professorships play a critical role at Rochester, as they allow the Chemistry Department to support the recruitment and retention of exceptional senior faculty. They also are crucial to expanding the reach of the Department into novel areas of Chemistry research. I want to sincerely thank everyone who has generously donated over the many years to support the Kende and Eisenberg funds, which have led to the creation of the Eisenberg and Kende endowed Chairs in Chemistry, respectively. Stay tuned... as we hope to have major announcements on these Professorships in the coming months.

I want to thank all of our alumni for your continuing and generous support of the Department for the past year. You provide critical feedback into how to best advance Chemistry at Rochester and we appreciate the input. Our "Chemistry Alumni Research Fund" is a great resource for the Department as it enables us to pursue a number of impactful endeavors, including this year being used to support over two dozen Fellowship awards to support graduate student research, education, and travel. Unlike the "Dean's Fund for Chemistry," which is not under the purview of the Department and is primarily used to supplant the College's expenses for ongoing Chemistry activities by the Dean of the College, the "Chemistry Alumni Research Fund" is under Departmental control and gives us additional resources we can leverage to the advantage of the faculty and students in the Department.

Finally, I wish to extend a personal invitation to return to Rochester for Meliora Weekend in 2019, with events running from Thursday October 3rd through Sunday the 6th. We will host the annual Chemistry Department Gates Happy Hour on campus in the late afternoon on Saturday October 5th of Meliora Weekend. The Gates Happy Hour provides a special opportunity to acquaint yourself with current members of the Department and reconnect with old colleagues and classmates. I also want to invite any alumni and friends of Rochester to attend our reception at the ACS meeting in San Diego in August on Monday the 26th. Please email Lynda McGarry at mcgarry@chem.rochester.edu for more information.

Best wishes for a healthy and rewarding next 12 months. Meliora!

Sincerely,

Todd D. Krauss

Professor of Chemistry and Chair

U D Remss

Professor of Optics

GIFTS OF \$50,000+

John L.Barg (B.S. '46) and Doris Barg

GIFTS OF \$25,000+

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Dr. Thomas J. Perun (Ph.D. `63)

Laura and Elliot Richman Travel

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In Memoriam

The Department of Chemistry mourns the passing of:

Bruce Ackert (B.S. `60)

Don Batesky (Sr. scientist)

Dr. Robert Michael Bilotta

(M.S. `78, Ph.D. `81)

Dr. David P. Brust (Ph.D. `65)

Dr. Wade Lee Callender (Ph.D. `51)

Dr. William Connick (FLW `98)

Dr. Alex D. Cross (FLW `57)

Dr. G. Graydon Curtis (B.S. `58)

Dr. Luis Alfredo Gomez

(M.S. `85, Ph.D. `90)

Dr. Robert Daulton Guthrie (Ph.D. `63)

Madeline Haft (Goldstein)

(B.A. `50, M.S. `57)

Dr. Donald Philip Harnish (Ph.D. '48)

John Oliver Helling (B.S. `57)

Elaine Hey (Burk) (B.A. `47)

Dr. Eleanor Humphrey (Nicholson)

(B.A. `37, M.D. `41)

Dr. Robert T. Jacobsen (B.A. `58)

Dr. Andrew Kende (Emeritus faculty)

Charles M. Kretchman (M.S. '39)

Dr. Marvin R. Lamborg (B.S. `51)

Dr. Arthur Howard Lerit (M.S. `69)

Dr. George W. Luckey (Ph.D. `50)

Paul T. MacGregor (B.S. `53)

Jean H. Marshall (Hofferbert) (B.S. `46)

Dr. Robert B. Martin (Ph.D. `53)

Dr. Joseph Timothy Mullhaupt (B.S. `54)

Dr. William H. Pirkle (Ph.D. `64)

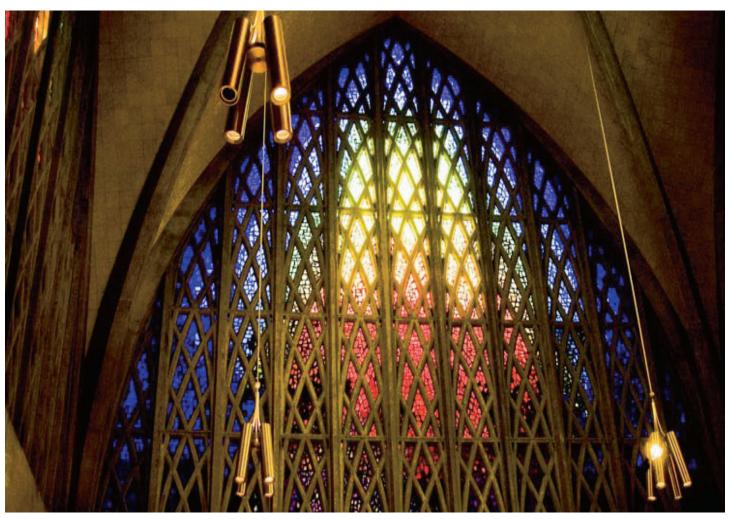
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Dr. Anne Turner (Halligan) (Ph.D. `69)

Dr. Gilden R. Van Norman (B.S. `54)

Milada S. Vanselow (Steiner) (B.A. `52)



Meliora Weekend 2018

The annual 2018 Marshall Gates Happy Hour was held in the afternoon on Saturday, October 6th in the Havens Lounge of Wilson Commons. In order to increase attendance at this annual event, graduate students and postdoctoral fellows were invited this year, along with Chemistry alumni and faculty. It was a great opportunity for everyone to share stories and network while enjoying great hors d'oeuvres and adult beverages. We are looking forward to the next Marshall Gates Happy Hour which will take place on Saturday, October 5th, 2019. Please join us this fall!



L to R: Jennifer Le, Andrew Vander Weide, George Alachouzos, Jing Yuwen, Dylan Parsons, Astrid Olivares



L to R: Lauren Bolz, Yashika Sharma, Antonio Tinoco



L to R: Ajay Laxman Chandgude, David Vargas, Juan Sebastian Sandoval



Caleb Whittier (`18) and Todd Krauss



Richard (`79) and Barb Aigen



Ignacio Franco and Dave McCamant



Alexandra Lahr, David Lahr (`98), Jim Farrar

Krugh Retirement

On Saturday May 5, 2018, a retirement party/birthday celebration was held for Tom Krugh at Next Door Bar & Grill in Pittsford, NY.









































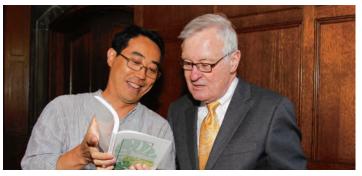


Farrar Retirement

On June 15, 2018 a symposium was held at the University of Rochester to celebrate the retirement of Professor Jim Farrar, and it was followed by a dinner party at the Memorial Art Gallery







Symposium Presenters:

Dwayne Miller- Max Planck Institute for the Structure & Dynamic of Matter

Cheuk-Yiu Ng- UC Davis

Franco Vecchiocattivi- Instituto per le Tecnologie Chimiche Universita di Perugia

Michael Carpenter- SUNY Polytechnic Institute Marty Zanni- University of Wisconsin Madison Charles Schmuttenmaer- Yale University Jim Farrar

Tom Rizzo- EPFL Laboratory of Molecular Physical Chemistry - Switzerland

Steve Sibener- University of Chicago **John Muenter-** University of Rochester

Stefano Falcinelli- Universita degli Studi di Perugia

Floyd Davis- Cornell University



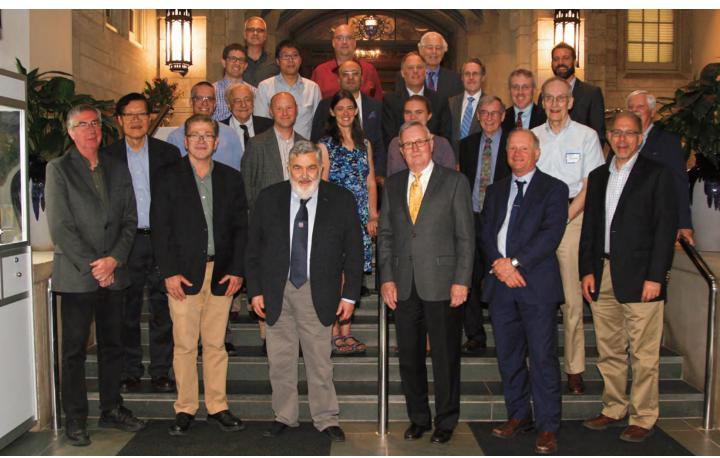


















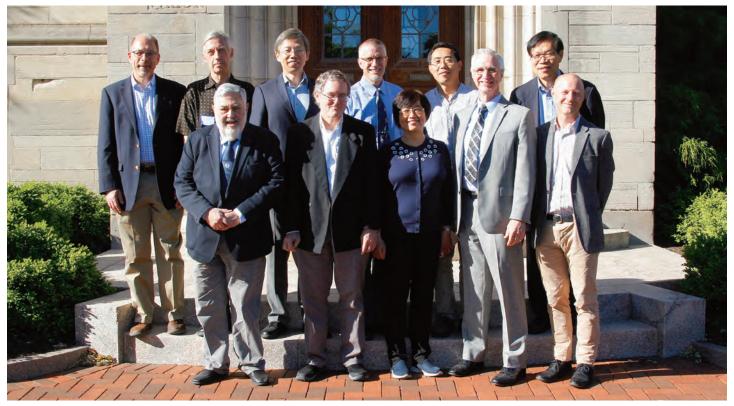
















Eisenberg Symposium

On August 21, 2018 the "Water Splitting & Solar Fuels: Progress & Challenges to Widespread Utilization" symposium was held in Boston honoring **Rich Eisenberg**, followed by a special dinner, all of which took place during the Fall 2018 ACS meeting.

















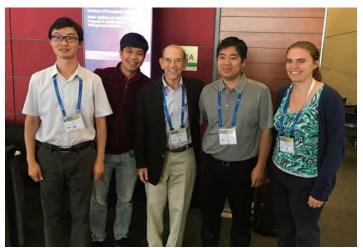














Faculty Awards

AWARDS

Kara Bren named a Fellow of the American Association for the Advancement of Sciences



Dr. Kara Bren has been named a fellow of the American Association for the Advancement of Sciences (AAAS). She was among 416 members of the association being recognized for their "efforts toward advancing scientific applications that are deemed scientifically or socially distinguished."

Fellows were selected for diverse accomplishments that include pioneering research, leadership within their field, teaching and mentoring, fostering collaborations and advancing public understanding of science.

Her other awards include an Alfred P. Sloan Research Fellowship and a Kavli Fellowship from the National Academy of Sciences. She is also a 2017 recipient of the University's Edward Peck Curtis Award for Excellence in Undergraduate Teaching.

Much of Kara's research has involved cytochrome c, a metalloprotein that, depending on how it is "folded," can either play a role in respiration or in apoptosis – the natural death of cells that occurs as part of normal growth. Working with colleagues in her department, she is exploring how derivatives of cytochrome c can be used as catalysts to produce hydrogen from water as a carbon free source of energy.

In addition to Kara's projects that have been funded by the NSF and the Department of Energy, Kara is also the Program Director for the recently awarded NIHfunded Chemistry-Biology Interface (CBI) Training Program. The overall goal of the program is to prepare predoctoral graduate students for productive and fulfilling careers in science. Activities in this program will help trainees develop skills needed in a range of careers in science, which includes scientific writing, giving effective presentations, and networking.

Pengfei Huo receives 2018 NSF CAREER Award



Assistant Professor **Pengfei "Frank" Huo** is the recipient of a 2018 CAREER Award from the National Science Foundation for his proposal "Quantum Dynamics of Photochemical Reactions in Solar Energy Conversions."

The Faculty Early Career Development (CAREER) Program is a Foundation-wide program that offers the NSF's most prestigious awards in support of junior faculty who exemplify the role of teacher-scholars through outstanding research, excellent education and the integration of education and research within the context of the mission of their organizations. Such support is expected to help build a firm foundation for a lifetime of faculty leadership in integrating education and research.

Huo and coworkers plan to develop new quantum dynamics approaches for investigating photochemical reactions. These reactions are crucial for solar fuel production. In solar-to-fuel reactions, a molecule is excited by absorption of light, and this process allows the molecule to transfer both electrons and protons to another molecule. A quantitative and predictive understanding of these reactions is hampered by the lack of efficient and accurate theoretical approaches. The Huo group will investigate new quantum dynamics methods that aim to address these theoretical challenges. They use computational tools to simulate coupled electron and proton transfer reactions in photocatalytic conversions. Such insights inspire new design principles and paradigms for next-generation photocatalytic energy production. Dr. Huo's research program is integrated with an educational component centered on theoretical chemistry, including the 'Journey to the Molecular World' summer school for high school students in the Rochester City School District. This project aims to inspire student curiosity and enthusiasm about molecular science and encourage high school students to pursue higher education in STEM topics.

Frank received his B.S. in chemistry from Lanzhou University of China in 2007. He then moved to Boston University to pursue his Ph.D. in theoretical chemistry with David Coker. Frank's Ph.D. work focused on developing efficient and accurate non-adiabatic dynamics methods to understand the excitation energy transfer process and the electronic coherence in natural light harvesting systems. In 2012 he joined CalTech as a postdoctoral researcher in the group of Tom Miller where he worked on extending the linearized pathintegral method to simulate the electron and excitation transfer dynamics, as well as applying a variety of novel computational methods such as ab-initio molecular dynamics tools and wavefunction-in-DFT embedding approach to explore the fundamental aspects of electron and proton transfer mechanisms in cobaltbased hydrogen evolution catalysts.

Ellen Matson Honored for Innovative Teaching and Research

In Fall 2018, Assistant Pofessor Ellen Matson was chosen as a Scialog Fellow for Advanced Energy Storage by the Research Corporation for Science Advancement (RCSA). RCSA is a foundation providing catalytic and opportunistic funding for innovative scientific research and the development of academic scientists - advancing American competitiveness in science and technology. This Scialog initiative involves annual meetings which are attended by about 55 early career Scialog Fellows and 10 distinguished scientific leaders in the field of energy storage, with the goal of identifying bottlenecks, finding avenues for breakthroughs, and building new scientific teams to pursue these ideas.

Dr. Matson was also selected as the winner of the **2018 Edith Flanigen Award.** The Edith Flanigen Award is conferred annually by the Collaborative Research Centre (CRC) 1109 to an exceptional female scientist at an early stage of her career for outstanding results on metal oxide water systems. The CRC 1109 at Humboldt-University of Berlin aims at the fundamental, molecular understanding of the interactions between selected

oxides and water. The award provides financial support of 15,000 Euro and was created in honor of Edith Flanigen who performed groundbreaking work on molecular sieves at a time when women were rarely found working in highly complex scientific careers.

Dr. Matson was one of five inaugural recipients of the Course Hero-Woodrow Wilson Fellowship for Excellence in Teaching. Created by Course Hero, an online learning library, and administered by the Woodrow Wilson National Fellowship Foundation, the \$40,000 fellowships are intended as "genius grants" for young, tenure-track scholars who strike a balance between research excellence and commitment to innovative, effective teaching practices.

Dr. Matson studied chemistry and science education at Boston University, graduating, with honors, in 2009. Her Ph.D. work was conducted in the laboratory of Suzanne C. Bart at Purdue University, where she studied the synthesis, characterization and reactivity of low valent uranium alkyl complexes. Following completion of her degree in 2013, Dr. Matson moved to the University of Illinois at Urbana Champaign, where she conducted postdoctoral research in the laboratory of Alison R. Fout investigating the design of redoxactive secondary coordination spheres for the activation of small molecules. For her excellence in graduate and postdoctoral research, Dr. Matson was awarded the Iota Sigma Pi Anna Louise Hoffman Award for Outstanding Achievement in Graduate Research (2013) and the American Chemical Society Division of Inorganic Chemistry Young Investigator Award (2014). In 2015, Dr. Matson started her independent career at the University of Rochester. In 2017, Dr. Matson was named the recipient of a NSF CAREER Award.



Ellen Matson (in center) receiving the Edith Flanigen Award in October 2018 at Humboldt University of Berlin.

CBI Training Program

The Chemistry-Biology Interface (CBI) Training Program and Retreat



L to R: Randy Schekman, Sabeeha Merchant, Chris Striemer, Kara Bren, and Sarah Bowman

We were delighted to learn in July 2017 that the NIH had awarded the University of Rochester River Campus with its first T32 grant to start a Chemistry-Biology Interface (CBI) Training Program for graduate students in the chemical and biological sciences. Science at the chemistry-biology interface applies chemical concepts and approaches to gain a better understanding of biological phenomena and human disease.

Chemistry Professor Kara Bren is the Program Director, and Professors Rudi Fasan and Bradley Nilsson are co-Directors. Lynda McGarry is the CBI

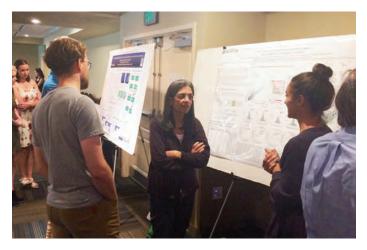
program coordinator. Thirty faculty members from six departments and programs in Arts, Sciences and Engineering and in the School of Medicine and Dentistry (SMD) serve as mentors to students participating in the CBI training program.

The overall goal of the CBI T32 program is to prepare predoctoral graduate students for productive and fulfilling careers in science at the chemistry-biology interface (CBI). The training includes coursework on CBI science, in critical thinking, and in effective scientific communication. Trainees participate in career development workshops that hone networking skills and that provide training on entrepreneurship and intellectual property. To develop leadership and group-work skills as well as teaching skills, trainees receive specialized training to serve as Peer-Led Team Learning (PLTL) workshop leaders for CBI courses.

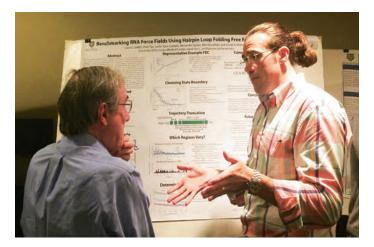
In this second year of the five year training grant, two trainees were recruited from the associated degree programs, which are Biology, Biomedical Engineering, Biochemistry, Biophysics, Chemistry, Microbiology and Immunology. These trainees are usually rising second-year students and they will be supported for 24 months provided strong progress is made after the first 12 months. For more information, please see the link on the Chemistry Department home page.



L to R: Arica Vanderwal, Shukree Abdul-Rashed, Emily Edwards, Dr. Kara Bren, Eric Moore, Clyde Overby, and Chapin Cavender









The Chemistry Department currently has two graduate students in the program; **Shukree Abdul-Rashed** is in Professor Alison Frontier's research group, and **Emily Edwards** is a member of the research group of T32 program director Chemistry Professor Kara Bren. **Arica Vanderwal** is a member of Professor Mitchell O'Connell's group in the Biochemistry and Biophysics Department in the medical center, and **Clyde Overby** works in the research group of BME Professor Danielle Benoit.

The two new trainees, Arica Vanderwal and Emily Edwards, joined two of the previous trainees Shukree Abdul-Rashed and Clyde Overby in the program. Eric Moore and Chapin Cavender, the third year trainees that joined the program for the first year only, continue to attend lunch meetings and other T32 activities and workshops.

The Biological Chemistry Cluster, formed in 2003, has actively worked to promote science at the CBI at UR and to foster interactions and collaborations benefiting CBI research. Faculty from SMD contribute lectures in chemistry courses and take a role in recruiting students interested in CBI research to the Chemistry PhD program. The highlight of the Cluster's activities is its annual retreat, which commenced in 2005.

The 2018 CBI Retreat was held on August 16th and 17th and the first keynote speaker on thursday was **Professor Sabeeha Merchant** from the UCLA Department of Chemistry. The title of her talk was "From Economy to Luxury: Mechanism of Eukaryotic Copper Homeostasis." The second keynote speaker was 2013 Nobel prize winner **Professor Randy Schekman** from UC Berkeley. His talk was entitled "RNA Sorting into Exosomes Secreted by Human Cells."

The second day of the retreat, attended by 70 participants, was held at The Staybridge Suites, and included a talk by **Dr. Sarah Bowman** from the Hauptman-Woodward Medical Institute. **Dr. Bowman** also participated in the career panel discussion with **Dr. Chris Striemer** (Adarza Biosystems), and our keynote speakers **Dr. Sabeeha Merchant** (UCLA), and **Dr. Randy Schekman** (UC Berkeley).

This lively and interesting discussion was followed by lunch, a poster session, and talks by graduate students **Eric Moore** (Fasan Group), **Chapin Cavender** (Mathews Group), **Jade Welch** (Nilsson Group), and **Christine Lai** (Ermolenko Group).

Magomedov Award

Dr. Neal Devaraj receives the 2018 Magomedov-Shcherbinina Award

The 2018 Magomedov-Shcherbinina Memorial Prize and Lectureship was awarded to **Dr. Neal Devaraj** on September 19th, 2018. The title of his seminar was "**Peering into the Lipid World.**" Dr. Deveraj received a dual B.S. in Chemistry and Biology from the Massachusetts Institute of Technology and his Ph.D. in Chemistry from Stanford University. After a postdoctoral position in molecular imaging at the Harvard Medical School, he joined the faculty of the University of California, San Diego in 2011, where he is currently a professor of Chemistry and Biochemistry. His research focuses on the design of bioconjugation reactions for addressing problems in bottom-up synthetic biology and cellular imaging. He is the recipient of the 2017 ACS Award in Pure Chemistry and the 2016 National Fresenius Award. He was recently named the 2018 Blavatnik National Laureate in Chemistry.

The Devaraj Lab at UCSD focuses on the design of chemoselective reactions for addressing problems in bottom-up synthetic biology and molecular imaging. Bioconjugation chemistries are some of the most important and commonly used tools in chemical biology. Their interdisciplinary research aims to advance



Dr. Neal Devaraj

important knowledge in chemical biology by extending the use of bioconjugation reactions into previously unexplored frontiers and challenging preconceived notions of where chemical reactions can be performed

This prize memorializes the lives of Nabi, Natalya, and their three year old son Amir Magomedov who lost their lives in a 2006 multi-vehicle accident. Nabi Magomedov was born on March 31, 1970 in Buynaksk, Russia, where his sister and parents still reside. He met his wife, Natalya, while studying at St. Petersburg University in Russia, where he earned his bachelor's and master's degrees in Chemistry. In 1995, he came to the United States to pursue his graduate education in chemistry at Ohio State University. Nabi completed his doctoral studies under the direction of Professor David J. Hart, receiving his Ph.D. in 2000, followed by postdoctoral research under the direction of Professor David Evans at Harvard University from 2000-2002.



In July of 2002 Nabi was appointed Assistant Professor of Chemistry at the University of Rochester. He was the recipient of several young investigator awards, including the Amgen New Faculty Award and the Research Corporation's Research Innovation Award.

Natalya joined Nabi in Columbus, OH in 1996 where she continued her studies at Ohio State University, earning a second master's degree. In March 2004, she joined Bausch + Lomb's surface sciences group, where she led the microscopy program. Natalya's passion for chemistry was surpassed only by her devotion to family. Amir Magomedov was born in Rochester, New York on November 24, 2002, the firstborn son of Nabi and Natalya.

REU Program 2018

During the spring and summer, **Professor Tom Krugh**'s main project involves organizing our NSF-supported **Research Experience for Undergraduates (REU)** program with the expert assistance of **Evelyn Sucy-Caffery.** During summer (2018) we had 20 undergraduates participating in the REU program. Our REU program reflects support for undergraduate research by faculty, the Chemistry Department, and the College. Undergraduate research provides an opportunity for graduate students (and postdocs) to gain leadership experience through one-on-one mentoring of undergraduates, both in the summer and during the school year. Mentors often describe their experience as important milestones in their graduate career.



Summer 2018 REU Poster Session participants (left to right, front to back):

1st Row: Suhyeon Kim, Aleksa Milosavljevic, Allison Stanko.

2nd Row: Jonathan Nadraws, Diego Garay, Maria Camila Aguilera-Cuenca, Chris Thaine, and Michela Maiola

3rd Row: Tiana Rohe, Jana Jelusic, Johnathan Negron Villalba, Gabriel Santiago Martinez Alvarez, John W.S. Clay,

Robert Love

4th Row: Karla Rosalia Sánchez Liévanos, Jisoo Woo

5th Row: Noah Gubernick, Garrett Hoteling, Aleksa Radovic, Jarrett Pelton

International Student Research Program

Since 2015 the Department of Chemistry has been hosting a Summer Research Fellowship Program designed to provide outstanding undergraduates in Chemistry from all over the world the opportunity to conduct first-class summer research at the University of Rochester. In this 2018 version, the Department invited seven students coming from very different parts of the world (Colombia, Mexico, Serbia, South Korea, and Spain) to join us for the summer. Through the program, these students receive a stipend to cover their living expenses and travel costs, and work closely with a faculty member in the Department for 8-10 weeks.

Photo below of the participants in the 2018 Summer Research Experience for Undergrads Program for International Students that Ignacio Franco coordinates, with many thanks to Barb Snaith and Evelyn Sucy-Caffery for their assistance.



2018 International REU Summer Students with graduate student mentors and faculty advisors

Back row: Ignacio Franco (Faculty Advisor), Lewis Rothberg (Faculty Advisor), Jeff Spears (Graduate Mentor), Aleksa Radovic (University of Belgrade, Faculty of Physical Chemistry, Serbia), Michael Neidig (Faculty Advisor), Jordan Andrews (Graduate Advisor), George Alachouzos (Graduate Advisor), Katie Knowles (Faculty Advisor)

Front row: Astrid Olivares (Graduate Advisor), Suhyeon Kim (KAIST University, South Korea), Gabriel Santiago Martinez Alvarez (Universidad del Valle Colombia, Colombia), Aleksa Milosavljevic (University of Belgrade, Faculty of Chemistry, Serbia), Diego Garay (University of Barcelona, Spain), Maria Camila Aguilera Cuenca (Nacional university of Colombia, Colombia), Karla Rosalia Sánchez Liévanos (Autonomous State University of Morelos ("UAEM") Mexico)

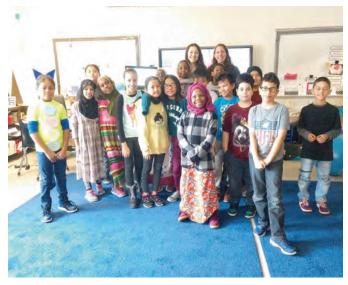
Student Outreach

Chemistry Graduate Student Association (CGA)



Eric Schreiber ('18, Matson Group), Brittney Petel ('15, Matson Group), Jacob Shelton ('17, Knowles Group), Emily Lasher ('18, Paradine Group), Melissa Koch ('17, Knowles Group), Rebeckah Burke ('14, Krauss Group), Trevor Tumiel ('17, Krauss Group), Antonio Tinoco ('15, Fasan Group), Shukree Abdul-Rashed ('16, Frontier Group), Nikki Wolford ('16, Neidig Group), Stephanie Carpenter ('14, Neidig Group) Not pictured: Abby Freyer ('13, Krauss Group)

CGA is a group of diverse graduate students, ranging from first year graduate students to fifth year graduate students. This year we were excited to welcome Eric Schreiber ('18, Matson group), Emily Lasher ('18, Paradine group), Jacob Shelton ('17, Knowles group), Melissa Koch ('17, Knowles group), Trevor Tumiel ('17 Krauss group), and Brittney Petel ('15, Matson group).



Brittney Petel and Tarah Dibenedetto teaching Rochester City School District students how chemistry is "Out of this World!"

The Chemistry Graduate Student Association (CGA) has the unique opportunity to be a mediator between the graduate students and faculty in the Department of Chemistry at the University of Rochester. As an organization it is our goal to open this line of communication, as well as plan academic, social, and outreach events for the department. In this past year, we have been able to substantially increase the community outreach within the department and organize both academic and social outings for the graduate students. In June, the department was involved in the Teachers' Challenge 5K to benefit the Rochester City School District. We had several department members walk and run, including many that placed!



UR Chemistry had several students, post-docs, professors, and staff participate in the Teacher's Challenge 5K at Durand Eastman Beach Park over the summer, raising money for the Rochester City School District.

We also had the opportunity to organize National Chemistry Week for the department in the fall of 2018, where we were able to reach over 500 Rochester City K-6 students and show them how Chemistry is Out of This World! CGA also hosted new social events like graduate student movie nights, watching movies such as Hocus Pocus and Die Hard. CGA is looking forward to growing in 2019 and have several new and exciting events planned!

Student Outreach

Early Connection Opportunity (ECO) Summer Program



Early Connection Opportunity program - a bridge program between high school and university that is designed to start students off in the right direction. Operating within the Office of Minority Student Affairs (OMSA), the program runs for four weeks, during which time the students live on campus and take a full course load to prepare them for their first semester at UR. For the past three years, the Chemistry Department has participated in this excellent program, with a chemistry lecture course being created and taught by graduate student Lauren VanGelder. The course content is structured to prepare the scholars for their UR general chemistry course; it consists of lecture four days of the week, workshops twice each week (lead by teaching assistants Shukree Abdul-Rashed and Jordan Andrews),

and one laboratory experiment. As a result of the program, ECO scholars are well prepared to take on their undergraduate studies at UR.

Special thanks to the Chemistry Department for providing lab coats and safety glasses to the scholars!

Horizons at Warner Summer Program

During the summer of 2018, several graduate students from the Chemistry Department participated as volunteers for the annual **Horizons at Warner Summer Program**. The Horizons Program is a high quality academic enrichment program for low-income K – 8th grade students from the Rochester City School District that takes place each summer on the University of Rochester Campus. The students experience a non-traditional school setting on our university campus for six weeks. A notable approach of the Horizons program is that it provides opportunities for blending academics with arts, sports, cultural enrichment, field trips, and confidence-building activities.



ECO Chemistry faculty: Lead instructor Lauren VanGelder (center), along with teaching assistants Shukree Abdul-Rashed (left) and Jordan Andrews (right).





Twice each week for the duration of the program, the Horizons students attended chemistry workshops designed by our chemistry department volunteers. Organized by graduate student Lauren VanGelder, volunteers designed interactive workshops which included demonstrations and classroom learning, as well as hands on experiments in our UR chemistry labs. Workshop themes covered all areas of chemistry, ranging from acid-base chemistry, to the chemistry of colors, to even a CSI-chemistry themed mystery!

In Summer 2018 the Horizons chemistry workshops had a record breaking number of volunteers, all of whom had a great time gaining teaching experience and giving back to the Rochester community and to the students!





2018 Horizons volunteers (left to right): Sreyoshi Sur, Kylie Ritz, Lauren VanGelder, Brittney Petel, Antonio Tinoco, Andy VanderWeide, Brad Schurr, Albert Nam, and Alex Fertig. Volunteers not pictured: Patrick Forrestel and Jordan Andrews

New X-ray Diffractometer

Department Receives Funding for a New X-ray Diffractometer



The chemistry department recently received funding for a new X-ray diffractometer from the NSF's Major Research Instrumentation (MRI) program. The principal investigator on the proposal, Professor William Jones, along with co-investigators Professors Rich Eisenberg, Ellen Matson, Michael Neidig, and Daniel Weix, successfully demonstrated the current need for this new instrument in support of their respective research programs. Additional strong contributions to the proposal came from Professor Kathryn Knowles and crystallographer Dr. William Brennessel. Rounding out the team was Ms. Debra Haring, whose superb technical expertise with grant proposals made for a smooth process.

Purchased in late 2017 and housed in the X-ray Crystallographic Facility in B04 Hutchison Hall, the new instrument has been operational for over one year now. After careful consideration the department chose a Rigaku Synergy-S diffraction system, equipped with



Graduate students Theresa Boddie and Stephanie Carpenter mount and center a crystal in preparation for data collection.

dual Cu and Mo microfocus X-ray sources, a HyPix-6000HE HPC detector, and a Cryostream 800 temperature controller. The instrument capable of collecting complete data for publication in as little 10-20 minutes, although most small molecule experiments take 1-4 hours. For times when the queue is long, two to three data collections per day are not unusual. Identification of substances can occur within minutes. In addition to the fast turnaround, the new instrument is able to produce P1 Fe1 P3 Fe2 P3 N6 N6 N7 N4 O2 C11 C12

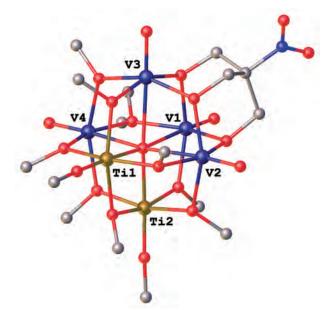
Crystal structure from Neidig group (https://doi.org/10.1021/jacs.9b05269)

high quality data on small powder samples and efficiently collect data on small macromolecules or preliminary data for larger proteins. Perhaps the most amazing capability is its ability to yield high quality structures from extremely tiny crystals, ones that were unable to be examined on the old instrument.

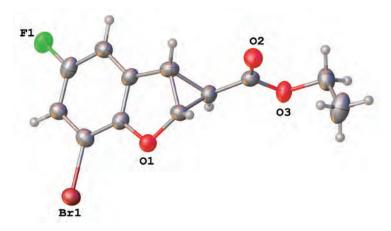
The obtaining of funding for the new instrument is only half of the success story. The usage statistics tell the rest. The number of publishable crystal structures has increased by 180 % from calendar year 2017 (old instrument) to 2018 (new instrument), and that for structures of strictly organic molecules has gone up by 750 %. The huge increase of the latter is due in large part to the ability to work with smaller crystals.

Students and researchers are fully trained on the diffractometer by taking graduate level course CHM 416, X-ray Crystallography. Additionally, undergraduate students are introduced to the instrument during a laboratory session in CHM 234, Advanced Laboratory Techniques. As part of the outreach program, researchers at local colleges and universities can submit samples for pro bono analysis. In many cases crystal structures are essential to achieving publication of their work or they allow the work to be reported in higher echelon journals. Samples from researchers at more distant colleges, universities, and other non-profit organizations are also accepted.

Details about the new X-ray diffactometer and specific experiments can be found at www.chem.rochester. edu/~xray. For additional queries, please contact the staff at xray@chem.rochester.edu.



Crystal structure from Matson group (https://doi.org/10.1016/j.poly.2019.04.022)



Crystal structure from Fasan group (https://doi.org/10.1002/anie.201903455)

Chemistry Welcomes Shauna Paradine

Assistant Professor of Chemistry

Ph.D. 2015, University of Illinois, Urbana-Champaign



RESEARCH INTERESTS

Development of chemo-, site-, and stereoselective C-C bond-forming reactions via transition metal catalysis for the synthesis of topologically complex organic scaffolds, discovery of novel transition metal catalysts, synthesis of biologically relevant sp3-rich organic molecules

CONTACT sparadin@ur.rochester.edu

SHAUNA PARADINE joined the Chemistry faculty in July 2018. A native of southwest Michigan, Shauna earned a B.A. in chemistry from Albion College in 2008, where she performed research under the guidance of Prof. Andrew N. French. She pursued her graduate studies in the group of Prof. M. Christina White at the University of Illinois at Urbana-Champaign as a NSF Graduate Research Fellow. Her Ph.D. research focused on

pioneering the development of site- and chemoselective iron- and manganese-catalyzed C(sp³)—H amination reactions. After completing her Ph.D. in early 2015, Shauna moved on to Prof. Eric N. Jacobsen's lab at Harvard University, where she was a NIH Postdoctoral Fellow. Her research there entailed the use of cocatalysis with chiral dual hydrogen bond donors for the development of chemo- and enantioselective multicomponent reactions.

Shauna is excited to begin her independent career at Rochester and to contribute to the world-class teaching and scholarship for which the University is renowned. Three talented first-year graduate students joined the group in December, ready to jump-start her research program: **KAIT HOUGHTLING, EMILY LASHER,** and **JAKUB VAITH.** Another welcome addition was **PAT HARRINGTON** (Ph.D. '18, with Alison Frontier), who joined the group as a postdoctoral fellow in January.

During the fall semester, Shauna taught Organic Reactions (CHM 435), a graduate level course.

Selected Publications:

A Manganese Catalyst for Highly Reactive yet Selective Intramolecular C(sp3)—H Amination. Paradine, S.M.; Griffin, J.R.; Zhao, J.; Petronico, A.L.; Miller, S.; White, M.C. *Nat. Chem.* **2015**, 7, 987-994.

Iron-Catalyzed Intramolecular Allylic C–H Amination. Paradine, S.M.; White, M.C. J. Am. Chem. Soc. **2012**, 134, 2036-2039.

Catalytic Enantioselective α-Oxysulfonylation of Ketones Mediated by Iodoarenes. Altermann, S.M.; Richardson, R.D.; Page, T.K.; Schmidt, R.K.; Holland, E.; Mohammed, U.; Paradine, S.M.; French, A.N.; Richter, C.; Bahar, A.M.; Witulski, B.; Wirth, T. Eur. J. Org. Chem. 2008, 5315-5328.

Enantioselective α-Oxytosylation of Ketones Catalysed by Iodoarenes. Richardson, R.D.; Page, T.K.; Altermann, S.; Paradine, S.M.; French, A.N.; Wirth, T. *Synlett*, **2007**, 538-542.





Emily Lasher, Jakub Vaith, Kait Houghtling

Faculty News

Robert K. Boeckman, Jr.

Marshall D. Gates, Jr. Professor of Chemistry

Ph.D. 1971, Brandeis University



RESEARCH INTERESTS

Total synthesis of alkaloids, terpenes, antibiotics, and antitumor agents; development of new synthetic methodology including the asymmetric synthesis methods involving the Diels-Alder reaction, the Claisen-retro-Claisen and other reactions; applications of conformational theory to the development of stereocontrolled organic reactions.

CONTACT

rkb@rkbmac.chem.rochester.edu

During 2018, **ROBERT K. BOECKMAN, JR.** has been on Sabbatical leave since July 1, 2018 and has continued full time teaching and research. He also remains as President and Chair of the Board of Directors of Organic Syntheses, Inc. As of July 1, 2019, he will retire as Marshall D. Gates Jr. Professor of Chemistry, becoming Marshall D. Gates Jr. Professor of Chemistry, Emeritus.

The Boeckman research group forged ahead with their efforts directed toward the development of new synthetic methodology and the application of that methodology to problems of current interest in complex molecule synthesis, particularly molecules possessing important biological activity. Significant progress has been made in the past year toward the synthesis of FK-506, as well as projects directed toward Apoptolidin. New asymmetric spiroannulation chemistry has been developed and applied to a 2nd generation scalable synthesis of antitumor Manzamine class alkaloid (-)-Nakadomarin A. Significant improvements have been made both in yield and selectivity at several key stages of the synthesis. The group has also completed their first efforts in organocatalysis with the development of catalytic systems for hydroxymethylation of aldehydes. Studies in this area are continuing and have culminated in a new and more efficient and scalable synthesis of (-)Rasfonin which has shown promise for treatment of pancreatic tumors. Near



Venkat Srinivasan, Thomas Lyon (REU), Kyle Rugq, Don Batesky, Bob Boeckman, Justin Niziol, Noah Sims (REU), Dennis Savage

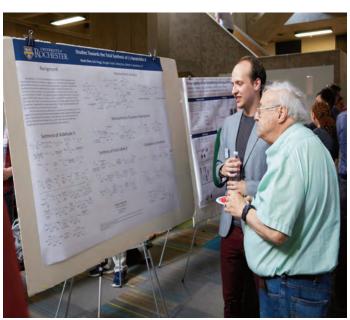
gram quantities have been obtained and the material has been submitted for evaluation by our colleagues at the Max Planck Institute of Molecular Physiology led by **PROFESSOR DR. HERBERT WALDMANN**. Collaborations continue with DR. HAL EBETINO (PH.D. '84) (Research Professor in Chemistry), and DRS. BRENDAN BOYCE and LIANPING XING of the URMC Department of Pathology and Laboratory Medicine which have resulted in the development of a Bone Targeted Drug Delivery Platform Technology. These include promising leads toward Bone Targeted Therapies for Bone Related Effects of Rheumatoid Arthritis, Osteoarthritis and Bone Cancer Chemotherapies. Lead compounds are being evaluated by G. David Roodman, Teresita Bellido and Jesus Delgado-Calle at the University of Indiana Medical School in Indianapolis. One of the leads against Multiple Myeloma is being licensed for development by Shenzhen Ionova Life Sciences Co., Ltd. Exciting new collaborations have been initiated with Professors Graham Russell and Raj Thakkar, and Dr. Udo Oppermann of the Nuffield School of Medicine at Oxford University UK.

KYLE F. BIEGASIEWICZ (PH.D. '16) remains at Princeton as a postdoctoral associate with Todd Hyster. **DOUG TUSCH**, who defended his thesis in March 2017, has assumed a lecturer position at RIT teaching laboratory courses. **LIFENG XIAO** defended his thesis in June 2017 and, after a postdoctoral year and a half at UC Berkeley working with Matt Francis, returned to China as a PI at Livzon, a pharmaceutical company in Zhuhai CN in Guangdong near Hong Kong. Sarah (Paulson) Madden joined the law firm LeClairRyan in

Bob and Mary at Jim Farrar's retirement and birthday celebration.

Rochester as Patent Technical Specialist. Postdoctoral associate VENKATESAN SRINIVASAN (PH.D. '09) continues the preparation of bone-targeted and receptor-targeted drug conjugates, and promising leads have been identified for treatment of bone resorption accompanying rheumatoid arthritis therapy, and multiple myeloma in collaboration with Dr. Hal Ebetino of Chemistry, and Drs. Brendan Boyce and Lianping Xing from the URMC. Fifth year student **KYLE RUGG** defended his thesis in November 2018 and in December he joined the Process Research Group at Boehringer Ingleheim in Ridgefield CT. Fourth year graduate student JUSTIN NIZIOL completed a new, scalable route to (-)-Rasfonin and is also carrying on the synthesis of FK-506, picking up where Kyle Biegasiewicz left off; an effort which is reaching the latter stages. Part-time scientist DR. DENNIS SAVAGE, retired from Kodak, continues his work in the group on several projects.

We will greatly miss the humor and chemical expertise of senior research associate **DON BATESKY** who passed away in September 2018. After retiring from Kodak, Don worked as a contract chemist for the Aldrich Company for 15 years. He spent many of those years working alongside two other former Kodak chemists in leased laboratory space in Hutchison Hall. After his contract with Aldrich expired, Don worked for four years in Dan Weix's lab. Since 2017, he had been splitting his 25-hour week working with Bob Boeckman and also with the Optical Materials Laboratory at LLE to synthesize a series of glassy liquid crystal (GLC) materials. Please see the tribute to Don at the end of this newsletter.



Bob discussing research with Noah Sims at the REU poster session.

Professor of Chemistry



RESEARCH INTERESTS

Bioinorganic and biophysical chemistry: engineered metalloprotein and metallopeptide catalysis for solar fuels, biological and nanotechnological systems for solar energy conversion, heme protein structure and function, protein dynamics.

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This past year brought progress in science and career development for the Bren group, with a new research direction in nitrogen cycle chemistry gearing up in the lab and new opportunities realized for current members and alumni.

The group was happy to welcome **JIWON HAN** as a new first-year graduate student. Jiwon joins us from Ewha Womans University in Seoul, after having done an iREU with the lab in the summer of 2017. Jiwon is doing electrochemical studies of cobalt peptide catalysts for hydrogen evolution from water. We also bid farewell to **YIXING GUO**, who successfully defended his Ph.D. thesis on electrocatalytic hydrogen production and has taken a position at Intel in Dailan, China. Yixing made this big move with his wife, **JING YUWEN** (Ph.D. from Jones this past year), and their new baby girl Harper.

Other members of the Bren group have been making use of electrocatalysis in their work. Fourth-year student **JENNIFER LE** published a paper in

Chemical Science on hydrogen production by a synthetic protein in collaboration with PROF. ANGELA **LOMBARDI** (University of Naples) and **DR. VINCENZO FIRPO** (University of Naples), a previous visitor to the lab. Jen won a Departmental Travel Award to present this work. She also has been mentoring UR senior REBECCA SHEETS ('19) in her senior project. Third-year student JOSE ALVAREZ-HERNANDEZ along with UR undergraduate ANDREW SOPCHAK ('20) have made great progress in understanding the mechanism of electrocatalytic hydrogen production by a cobalt porphyrin-peptide. Jose won a Carl Storm Fellowship to present his work at the Metals in Biology Gordon Research Conference. Third-year student JESSE STROKA has also been doing electrochemistry, but in a new effort to develop catalysts for the reduction of nitrite and nitrate to ammonia. Jesse worked with Yixing on this project and they published their first results in JACS.

On the photochemistry side of the group, senior group member **SAIKAT CHAKRABORTY** and undergraduate



The Bren Group (L to R): Jose Alvarez-Hernandez, Andrew Sopchak, Emily Edwards, Jana Jelusic, Kara Bren, Saikat Chakraborty, Jiwon Han, Jennifer Le, Jesse Stroka



The Bren Group looking festive for Jiwon's first group meeting presentation.

JANA JELUSIC ('20) have been working with BECKAH BURKE of the Krauss lab and ALEX FERTIG of the Matson lab on a collaborative project on photocatalytic hydrogen production using quantum dots and cobalt-based catalysts that form in situ. Together, this team has made strides toward understanding the complex chemistry of this system. Second-year student EMILY EDWARDS has also joined these efforts to understand photochemical hydrogen production, collaborating with Saikat on characterizing his biomolecular system for photochemical hydrogen and starting her own studies on mechanism of this system. We were very pleased that Emily was awarded an NIH T32 Traineeship in the Chemistry-Biology Interface program.

Kara enjoyed many travels and events in 2018. The highlight of her year was giving the KAIST (Korea Advanced Institute for Science and Technology) Lectureship in Daejeon, Korea. This visit included a talk and discussion on women in science, the first ever held for chemistry students at KAIST. She presented the group's new nitrogen cycle chemistry in talks at the Metals in Biology Gordon Conference in Ventura, CA, and as a Plenary Speaker at the Royal Society of Chemistry Dalton Division Meeting in Coventry, UK. She also learned a lot by participating in an electrochemistry workshop in Marseille, France, which is a center for bioelectrochemistry. Directing the NIH Chemistry-Biology Interface Training Program, she arranged a number of career development events for students including the annual retreat, none of which would have been possible without the support of Lynda McGarry. Kara also continued her work as an Associate Editor for IACS, assisted by Valerie Drake, after signing on again with ACS for a position that continues to challenge and stimulate.



The Bren Group hosting an "Ask a Scientist" booth at the Brighton Farmer's Market.

Joseph P. Dinnocenzo

Professor of Chemistry



RESEARCH INTERESTS

Chemistry of organic ion radicals; mechanistic and physical organic chemistry.

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JOE DINNOCENZO and his group continue to pursue a variety of problems in electron transfer chemistry and photochemistry.

The group has been exploring recently discovered cationic exciplexes that result from a charge-shift between cationic, excited state electron acceptors and neutral donors. We recently found that emissive cationic exciplexes can be formed in water which, to the best of our knowledge, are the first examples of emissive, organic exciplexes in water reported in the literature. Critical to the success of this project was the synthetic work of graduate student **ANALUZ MARK** who prepared organic cationic acceptors with neutral donors tethered to the acceptor via trimethylene chains. Interestingly, the cationic exciplexes in water were found to have relatively large quantum yields for emission and remarkably long lifetimes.

Dr. Adam Feinberg, center, with other researchers, including, from left, Evan Lloyd, Oleg Davydovich, Edgar Mejia and Sydney Butikofer. (Credit: Lyndon French for The New York Times)

In other work, **ANALUZ MARK** is continuing research on novel fragmentation reactions of Group 14 cation radicals and on the reactions of alkoxyl radicals as hydrogen atom donors.

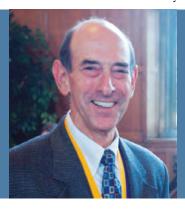
In group news, former graduate student **DR. MARY LENCZEWSKI**, who is a chemistry professor at Ohio University (Eastern), received tenure this past year. Congratulations Mary!! Former graduate student Dr. **ADAM FEINBERG** has enjoyed notable success in Prof. Jeffrey Moore's research group in the Beckman Institute at the University of Illinois at Urbana-Champaign. Adam's work on photodegradable polymers. His work was recently highlighted in a feature article in the New York Times. Way to go Adam!

Joe continues to enjoy working in the lab on a regular basis. He and **SAMIR FARID** have been working on several projects involving novel exciplex intermediates;

work that is funded by a recently renewed grant from the National Science Foundation.

Joe has also been collaborating with Dr. Cecilia Barone and her colleagues in Rochester's Center for Excellence in Teaching and Learning (CETL) on a project that uses live interactive theatre to train peer led team learning (PLTL) leaders in recognizing visible and invisible barriers to participation experienced by students in diverse STEM teams. We are now in the third year of this exciting project, which trained over 160 new leaders this past fall. In the future, hopefully with the assistance of a grant submitted to the NSF, we propose to create new theatre-based video resources that will use some of the elements of the live interactive theatre experience to train PLTL leaders both at Rochester and other institutions around the country.

Professor of Chemistry / Research Professor



RESEARCH INTERESTS

Inorganic and organometallic chemistry; artificial photosynthesis and light-tochemical energy conversion; complexes of the platinum group elements (PGE's) and gold; homogeneous catalysis; photochemistry and photophysical properties of metal complexes; oxidative addition and bond activation chemistry; use of luminescent complexes in light emitting diodes; parahydrogen induced NMR effects in hydrogen addition reactions.

CONTACT

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RICH EISENBERG writes that it has finally happened - his lab has closed after 45 years in Hutchison B-48 and nearby surroundings in the basement. It was a great run, but all good things must come to an end. What's more, he has new, bright colleagues with whom to talk chemistry and discuss what they are doing or planning to do. Rich's last two postdocs moved on to permanent jobs in 2018 - **HONGJING LV** returned to China under its Thousand Young Talents Program to a position at Beijing Technical University while **GUOCAN LI** took a position at a company in Pennsylvania.

Since the last Newsletter, Rich has been busy with various activities in science; he remains an Associate Editor of *PNAS*, and in Fall 2018, he organized a Sackler Colloquium under the National Academy of Sciences on the <u>Scientific Status and Challenges in the Decarbonization of Our Energy Landscape</u> among other activities. During 2018, Rich attended both ACS National Meetings for different celebrations and also gave several lectures including the Jonassen Lecture at Tulane and a talk at the Technical University of Denmark. The Spring 2018 ACS Meeting was in New Orleans and it included a celebration of a wonderful group of lifelong friends who turned 75 during the prior year. The group photo is shown below and contains Harry Gray (over 75) and Cliff Kubiak (well under 75). If you are chemistry savvy, see how many of the friends you can name! The celebration took place on St. Patrick's Day in the French Quarter and included wonderful food spiced by a heaping bit of rock and roll.

At the Boston ACS Meeting in August 2018, Kara Bren organized a symposium and dinner in honor of Rich, and at the dinner, Dean Gloria Culver announced the creation of the **Richard S. Eisenberg Professorship in Chemistry**. Fund-raising is continuing, but the goal is in sight, and it is a very special honor for Rich in recognition of his four-plus decades of service, teaching and research at Rochester. At his last DOE contractors' meeting, Rich chaired a session and then ended with thanks to all, followed by a dropped mic in the Obama tradition

Rich and Marcia will now spend most of their time in Sarasota, FL, while summering in Rochester. His focus is now on collision theory and momentum transfer over photosynthetically modified surfaces.



Rich and Marcia in Scandinavia



Rich and friends and colleagues at Spring 2018 ACS Meeting in New Orleans

Samir Farid

Research Professor



RESEARCH INTERESTS

Mechanisms and kinetics of photoinduced electron transfer reactions; fundamental aspects of ion pair dynamics and the kinetics of radiative and nonradiative electron transfer processes.

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SAMIR FARID enjoys his collaboration with Joe Dinnocenzo, which he finds stimulating and productive. During 2018, they built on their last year's discovery of a new class of exciplexes in which the acceptor is a cation resulting in

charge shift reaction, in contrast to the conventional exciplexes, which are charge formation reactions. Joe and graduate student **Analuz Mark** synthesized watersoluble, intramolecular analogues. These compounds were used to demonstrate that emissive, purely organic exciplexes can be formed in water. Extensive steady state and time-resolved investigations were used to probe the role of several conformers, through-bond electron transfer, and stereoelectronic effects. A detailed paper was submitted to J. Org. Chem. Samir continues a long-standing interest in Egyptology, and occasionally makes presentations on the subject at the Memorial Art Gallery.





Professor of Chemistry



RESEARCH INTERESTS

Dynamical studies of low energy ion-molecule reactions in the gas phase; imaging studies of collisions; photochemistry of size-selected ionic clusters.

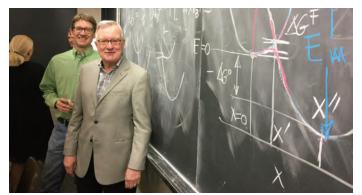
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The past academic year was Jim's last in the Department. In his final semester of teaching, he taught the second semester of "p-chem" on the subject of Thermodynamics, commenting that he felt that he had finally achieved some degree of understanding of the subject. Last June, Jim reached age 70, and decided that it was time to retire. The Department held a day-long symposium and dinner on his birthday. Many of his former graduate students and postdocs attended, and former faculty members **Tom Rizzo** and **Dwayne Miller** also came back to Rochester; please see the full article with pictures in this newsletter (page 15.)

Since then, Jim has given away much of his lab equipment, with the time-of-flight instrument going to **Floyd Davis** at Cornell, and the crossed beam instrument going to **Stefano Falcinelli** in Perugia. Stefano and Jim disassembled the machine in the summer of 2018, five crates of instrumentation sailed to Genoa aboard the container ship Brotonne Bridge in December, and just before Christmas, everything arrived in Perugia. In late Spring 2019, Jim will go to Perugia to help reassemble the crossed beam instrument, and, of course, enjoy the sights, the food, and the wine. Jim's wife, Kathy, says that he is not allowed in Italy without her!

After 42 years in Rochester, Jim expresses his gratitude to his colleagues in the lab and the Department for making Rochester such a special place. And of course, many generations of students in the classroom have made Jim's career so enjoyable and rewarding! Thanks to all of them!



Jim's last lecture



Jim with Stefano Falcinelli



Taking apart the crossed beam instrument



Container ship Brotonne Bridge

Associate Professor of Chemistry



RESEARCH INTERESTS

Bioorganic chemistry, biocatalysis, chemical biology; macrocyclic peptide inhibitors of protein-protein interactions; metalloenzyme design and engineering; biocatalytic C—H functionalization and carbene/nitrene transfer reactions; chemoenzymatic synthesis.

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PROF. RUDI FASAN and his group continue their research focused on the design and application of metalloprotein catalysts and chemoenzymatic strategies for late-stage C-H functionalization and asymmetric synthesis and on the development of new methodologies for the evolution of macrocyclic peptide inhibitors of protein-protein interactions. Over the past few years, our group has been engaged in developing new metalloprotein-based biocatalysts for abiotic carbene and nitrene transfer reactions. Expanding upon these efforts, postdoctoral fellow DR. AJAY CHANDGUDE has developed an efficient biocatalytic strategy for the highly diastereo- and enantioselective construction of nitrilesubstituted cyclopropanes via myoglobin-mediated carbene transfer catalysis (Angew. Chem. Int. Ed., 2018). This strategy provides a versatile approach to afford a variety of enantiopure cyclopropanes by combining enzymatic cyclopropanation with chemical manipulation of the nitrile group. In a collaborative effort with computational chemists and structural biologists, this past year we have gained key insights into the mechanism (J. Am. Chem. Soc., 2018) and the structural determinants underlying the high stereocontrol of an engineered myoglobin catalyst previously developed in the lab for stereoselective olefin cyclopropanation with diazoester reagents (ACS Catal., 2018). These studies, which were accomplished by graduate students ANTONIO TINOCO, VIKTORIA STECK, and ERIC MOORE, along with postdoc DR. DANIELA CARMINATI, have helped us paint a mechanistic framework for understanding the reactivity of these systems and guiding future catalyst development efforts. Eric and Viktoria have also reported success in developing a unique carbene transfer (bio)catalyst with high chemoselectivity toward promoting cyclopropanation in olefin substrates containing inherently more reactive Y-H bonds (Y = N, Si, or O) J. Org. Chem., 2018). This challenging task was realized through the use of a myoglobin catalyst with

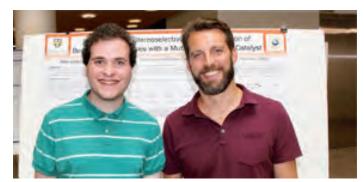
a redesigned cofactor environment featuring a nonnative metal center (Co instead of Fe) and first-sphere coordination residue (Ser instead of His). In the same vein, second-year graduate student DAVID VARGAS, along with Antonio and Vikas, have demonstrated the successful application of engineered myoglobins for the chemoselective C-H functionalization of unprotected indoles (Angew. Chem. Int. Ed., 2018). This method bypasses the need for protection/deprotection of the reactive N-H group typically required for C3functionalization of indoles via carbene transfer chemistry. Major progress in other projects within this area were also made by second-year graduate student **ALBERT NAM** and two talented postdoctoral fellows who have joined the metalloenzyme team over the past year: DR. DANIELA CARMINATI, who came to our lab with a background in metalloporphyrin chemistry from the Gallo group at the University of Milan (Italy), and DR. XINKUN REN, who completed his Ph.D. studies in P450 engineering/biocatalysis under the guidance of Prof. Luet Wong at Oxford University. Both have rapidly contributed to our research with manuscripts being in



Viktoria Steck, Antonio Tinoco and Eric Moore at the 255th ACS National Meeting in New Orleans

the works. This year the group bid a fond farewell to HANAN ALWASEEM (PH.D, '18), who defended her Ph.D. thesis in December and moved to the Big Apple after taking a scientist position at the Proteomics Center of Rockefeller University. In her final year in the lab, Hanan completed an insightful analysis of the anticancer activity of chemoenzymatic parthenolide analogs (Bioorg. Med. Chem., 2018) and completed a project focused on the thermostabilization of the multidomain P450 BM3 via directed evolution (Chembiochem, 2018). Hanan has also been the linchpin of a series of collaborative projects with the Ghaemmaghami group in Biology and the Benoit group in BME, which are currently being finalized for publication. The baton of our P450centered projects is now carried on by second-year graduate student ANDREW BORTZ, who is bringing this research in a new exciting direction, and by first-year graduate student ROBERT POTENZINO, who joined our group during the Fall.

Important strides forward were also made by the group members engaged in our peptide macrocycle projects. With the help of visiting student **KRITTIKA RALHAN**, postdoc **SACHINATAND MALI** has successfully developed a more potent cyclic peptide inhibitor of the Hedgehog pathway, which is aberrantly activated in a number of cancers. With seed support through a Technology Development Fund, the group is currently investigating the translational potential of these compounds. Our congratulations and best wishes go to **ANDREW OWENS (PH.D, '18)**, who completed his Ph.D. over the summer and left the team to join the R&D unit at Merck. Building upon Andrew's work, second-year graduate students **JAKE IANNUZZELLI**



Noah Gubernick and Rudi at the REU poster session

and **YU GU** are now spearheading our efforts in the development and application of high-throughput platforms for the evolution of macrocyclic peptide inhibitors of Hedgehog and other cancer-relevant target proteins. We also send our best wishes to Krittika, who ended her Nehru-Fulbright internship in the spring and returned to India to completing her Ph.D. and give birth to two beautiful twins. This past year Sachin was also blessed with the birth of a daughter, adding to the growing number of the lab's (grand)children.

lab celebrated several The other important accomplishments of current and former members of the group. TESSA BAKER (PH.D, '18), a joint graduate student with the Neidig lab, earned her Ph.D. in the summer and became manager of the NMR Facility in our department. After completing senior research in our laboratory, YASHIKA SHARMA (B.S. '18) graduated in May and is now a medical assistant at the URMC across the street. Other former undergraduate members of the group reaching this important milestone are **REBECCA** GALER (B.S. '18; now M.D. candidate at Virginia Commonwealth University), **HASSAN BEESLEY**



(B.S. '18; M.D. candidate at Boston University) and CHRISTOPHER PERALTA (B.S. '18), who has taken a staff scientist position at the Memorial Sloan Kettering Cancer Center. This past year we also bid a fond farewell to AGUSTINA VILA, a visiting UNESCO research fellow from the University of the Republic in Uruguay. Agustina will be soon be re-joined by Viktoria Steck, who will spend some time in the Carrera laboratory to conduct an NSF-supported collaborative project involving non-heme iron dioxygenases. Our group was happy to celebrate multiple awards bestowed to members of the lab in recognition of their excellent research and teaching accomplishments. These prizes include a Lattimore fellowship to Viktoria Steck, a Hooker fellowship to Eric Moore, and a Walters Teaching Award to David Vargas. Antonio Tinoco and Viktoria Steck also received travel awards from the ACS Division of Organic Chemistry and of Inorganic Chemistry, respectively, to present their results at the ACS Spring National Meeting in New Orleans. Last but not least, we were delighted about the award of the 2018 Nobel Prize in Chemistry to Dr. Frances Arnold, Rudi's postdoctoral advisor, for her pioneering contributions in the field of protein directed evolution.

The group has been also engaged in several important outreach activities. In commendable efforts led by Hanan, Antonio, Viktoria, and David, our laboratory hosted a dozen students and teachers from Brighton High School



Brighton High School students visit the Fasan Lab



David Vargas and the students during his outreach program in Colombia

to give them a taste of the type of work and activities conducted in a chemistry research laboratory. Kudos also go to David Vargas, who traveled to Colombia to participate in the Clubes de Ciencia (Science Clubs) outreach program and lead a week-long hands-on lab experience with a large group of high-school students, and to Antonio who participated and presented his research at the 2018 SACNAS Conference in San Antonio, Texas. During the National Chemistry Week, Hanan, Eric, Antonio, and David visited classrooms of an elementary school of the Rochester city school district to involve kids in fun workshops about the chemistry & geology of rocks. Finally, the group was happy to host **NOAH KUBERNICK** from RIT as a REU

fellow over the summer.

Over the past year, Rudi was promoted to the rank of Full Professor and he cherished the opportunity to talk about the research accomplishments of his group at various universities and meetings in the US and abroad. Among them, he enjoyed participating in a Summer School in Chemical Biology in Switzerland where he had the chance to interact with several students and scientists from across that country while being surrounded by spectacular alpine scenery. Over the summer, he and his family (Francesca, Penelope (6), and Matteo (5)) traveled to Italy for some restful family vacation during which they filled their days with making (and unmaking) sand castles, playing with marine organisms (alive and not), and taking swims in the warm waters of the Adriatic Sea.

Associate Professor of Chemistry



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.

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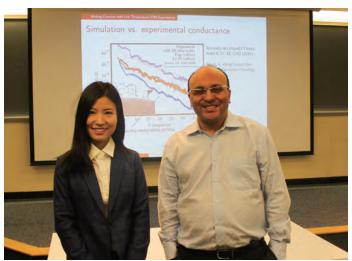
Using theory and computation, the Franco group investigates how molecules respond to external stimuli and how we can use that response as an active control tool to manipulate matter in intriguing and potentially useful ways. We tackle emerging problems at the interface between Chemistry and Physics, Optics and Nanoscience. We are engaged in active collaborations worldwide. We develop new theories, methods and computational algorithms. We strive to identify new phenomenology and new fundamental principles. We work closely with experimentalists, but we also like to be a few years ahead of experiments.



The Franco Group pumpkin carving

In the last five years in Rochester we have been tackling three central challenges in physical chemistry: 1) How do we control matter at the level of electrons using lasers? 2) How can we use non-trivial quantum mechanical effects to enhance molecular function? 3) How can we develop useful multidimensional spectroscopies that operate at the single-molecule limit? The group has been recognized by an NSF CAREER award and the ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry.

This has been an exciting year for us. Our postdoctoral fellow **DR. BING GU** received the 2018 PHYS Young Investigator Award of the ACS for his work in Rochester. Dr. Gu made beautiful advances developing theories for laser-dressed materials, general formulas for decoherence timescales, and understanding basic mechanisms for coherence loss. This award recognizes him as one of the top young researchers in Physical Chemistry in the nation. **ZHILI**, the senior Ph.D. student in the group, has now successfully defended her Ph.D. thesis "Frontiers in the Atomistic Modeling of Molecular Junctions: Bringing Theory Closer to Experiment" and published the first two papers of her Ph.D. work



Prof. Franco with Zhi Li

in top tier journals. WEN HU published his first paper investigating fundamental aspects of decoherence in molecules, gave his third-year presentation and is now a Ph.D. candidate in the material science program. ANTONIO GARZÓN published his first paper advancing schemes to control electrons in matter using few-cycle laser pulses, and successfully presented his 3rd year talk. He also received an international travel award to present his Ph.D. work. **LEOPOLDO MEJÍA** completed his M.Sc. degree and is now officially a Ph.D. candidate. He has now published his first two papers investigating the combination of mechanochemistry with molecular conductance. Because of his accomplishments, Leopoldo was awarded a Weissberger Memorial Fellowship for the 2018-19 academic year. During the summer we had the good fortune of hosting DIEGO **GARAY** from the University of Barcelona as part of our prestigious international REU program. During his stay, Diego investigated how chemical reactivity changes in nanoconfined environments.

Ignacio traveled extensively in the Spring to present the work of the group as part of his "tenure tour", and gave a talk in the Departmental colloquia in the Fall entitled "Molecules under Torture: Lasers, Forces, Voltages, and Beyond". The tenure tour included Physical Chemistry lectures at U. Southern California, U. Penn, UC San Diego, U. Illinois at Urbana-Champaign, Northwestern, Cornell, NYU, Duke, Boston/MIT/Harvard Theochem, U. Toronto, U. Chicago, U. Oregon, Yale, Stony Brook, Princeton, UC Irvine, U. Washington and U. Michigan! In addition, Bing presented 4 papers

of the group in the APS March meeting in Los Angeles, and one in the ACS Fall Meeting in Boston, and gave lectures in UC San Diego and UC Irvine. In the summer, Antonio presented his work in the 10th Photodynamics meeting in Cartagena (Colombia), and Ignacio and Leopoldo presented their work in the Gordon Research Conference on Donor-Acceptor Interactions.

During the summer, Ignacio organized an exciting Telluride workshop entitled "Quantum Frontiers in Molecular Science". He also led, for the fourth time, our prestigious i-REU summer research fellowship program for international students. This program is designed to provide outstanding undergraduates in Chemistry from all over the world the opportunity to conduct first class summer research at the University of Rochester. In the 4 years of this program the Department has hosted 24 extremely talented undergraduate students (coming from Brazil, Colombia (4), Cuba, Czech Republic, Germany, India (2), Italy, Korea (3), Mexico (3), Netherlands, Poland, Serbia (2), Spain, Sweden and the UK). Ignacio is very proud of this program as it has positively influenced the trajectory of very talented undergraduate Chemists by offering a key opportunity at the right time in their professional development.

In the Fall, Ignacio took a well-deserved break from traveling and did one of his favorite things in the world: teaching quantum mechanics in CHM251. It is always such a pleasure to guide our enthusiastic and talented undergraduate students into the conceptual depths and technical intricacies of quantum theory!



The Franco Group (L to R): Zhi Li, Diego Garay, Antonio Garzon, Bing Gu, Wenxiang Hu, Leopoldo Mejia Restrepo, Ignacio Franco

Professor of Chemistry



RESEARCH INTERESTS

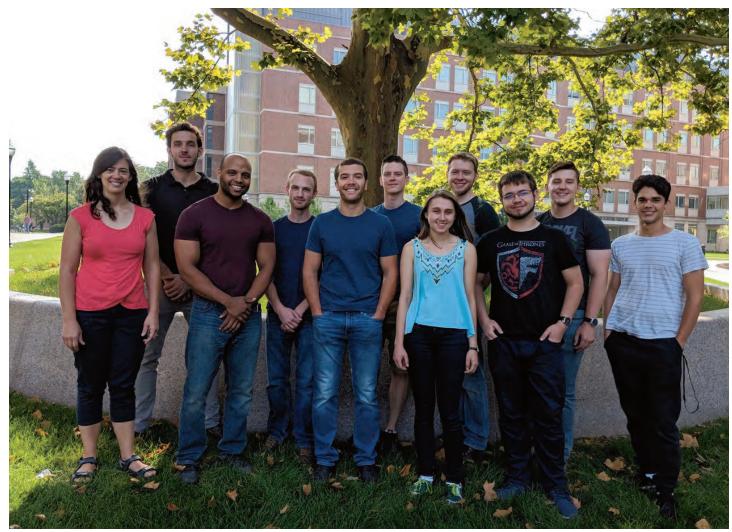
Synthetic organic chemistry; synthesis of bioactive natural products; pericyclic reactions; asymmetric catalysis; cationic cascades.

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. Our frustration with divinyl ketone precursors has taken us 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



The Frontier Group (L to R): Alison Frontier, Georgios Alachouzos, Shukree Abdul-Rashed, Connor Holt, Eric Stoutenburg, Dylan Parsons, Ally Stanko, Pat Harrington, Aleksa Milosavljevic, Rob Potenzino, Jackson Hernandez



Georgios Alachouzos, Jackson Hernandez, Dylan Parsons, Alison Frontier, Shukree Abdul-Rashed, Connor Holt

polycyclic molecules with embedded quaternary carbons. To these ends, we are hard at work developing a "carbonyl pinch" strategy that engages three simple precursors: an envne, a carbonyl building block, and a halide ion, which combine in a cascade sequence to produce complex halocyclopentenes (using "guess what" kind of reaction @). This chemistry was pioneered by GEORGE ALACHOUZOS (4th year), and CONNOR HOLT (2nd year) and JACKSON HERNANDEZ (1st year). DYLAN PARSONS (5th year) is developing cascade sequences of a different type, involving cation- π cyclization chemistry, and SHUKREE ABDUL-RASHED (3nd year) is studying alkynyl halo-Prins reactions and pursuing the synthesis of citridone A. Our bioactive natural product synthesis projects will continue in the context of the new strategies being developed in the lab.

In November and December 2018 we celebrated two successful Ph.D. defenses, which culminated in the

"crowning" of DR. ERIC STOUTENBERG, who is a scientist at Novomer, right here in Rochester, and DR. PATRICK HARRINGTON, who is now doing postdoctoral work with Prof. Shauna Paradine, again, right here in Rochester! We are glad they are still nearby for social events, or to help find something in the lab... This year, we welcomed JACKSON HERNANDEZ (B.S. 2018, University of Buffalo) to the group. We have four undergraduate colleagues working in the lab: **CULLEN WALSH ('19), ALISON STANKO ('19), BEN** LERNER ('19), and PAUL SINCLAIR ('20). Over the summer, we hosted ALEKSA MILOSAVLJEVIC, an undergraduate from the University of Belgrade, through the departmental international REU program. In the first photo, you see the lab in summer 2018. We had a mix of year-round group members, visiting undergraduates, and rotating graduate students. In the second photo you see a photo with graduate students only, with George Eastman on the quad on a wintry day.

Pengfei (Frank) Huo

Assistant Professor of Chemistry



RESEARCH INTERESTS

Physical and theoretical chemistry, Ab-initio dynamics for understanding chemistry and photo physics of solar energy conversion.

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The **HUO** group is developing new quantum dynamics approaches and investigating new chemical reactivities enabled by intrinsic quantum mechanical behavior.

Our *Annus mirabilis* continues in 2018, with various exciting news, including several publications and numerous awards for group members. We are also very honored to receive an EAGER grant and a CAREER award, both from the National Science Foundation to support the group's "quantum leap" into the new frontiers of Chemistry.

ARKAJIT MANDAL has published his trilogy (three back to back papers) on his wonderful idea, so-called quasi-diabatic representation. It aims to resolve a long-standing challenge in theoretical chemistry: the incompatibility between electronic structure methods and quantum dynamics approaches due to their different "footing". Arkajit has also made a wonderful contribution to our recent adventure on quantum



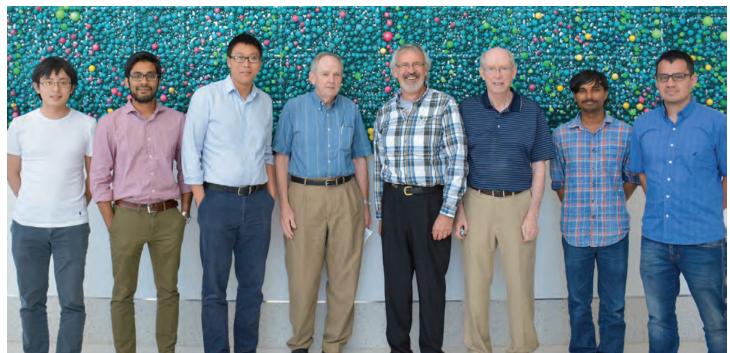
Arkajit Mandal receiving best poster award at CECAM

electrodynamics enabled chemical reactivities. This project has the potential to inspire transformative design principles that take advantage of intrinsic quantum behaviors of light-matter interactions and facilitate the quantum leap of chemistry. Arkajit had traveled to Lausanne, Switzerland, and Boston for conferences and won two best poster prizes. He also won a Weissberger Memorial fellowship because of his excellent academic and research achievements.

SUTIRTHA CHOWDHURY continues to develop his new theoretical approach that can provide a unified description for electron and proton transfer. With his hardworking efforts, he can now rigorously derive it from exact quantum correlation function. These works will soon appear as an invited contribution in a special issue on J. Chem. Phys. (special thanks to Prof. Michael Thoss). With his excellent research accomplishments and performance, Sutirtha won a Robert and Marian Deright Fellowship this year.

XINYANG LI continues his exciting project of using ab-initio quantum dynamics to investigate tunneling controlled chemical reaction. Some of his recent results are currently being prepared for publication. Xinyang as the "theory gadget wizard" is also providing excellent support to the computational chemistry classes and helping other graduate students to perform electronic structure calculations in the department.

This year, the group welcomes two new members. **DR. WANGHUAI ZHOU**, a lecturer at the Hubei University of Automotive Technology (China), joined our group as a Visiting scholar through the support of the China Scholarship Council. He is currently working on abinitio on-the-fly simulation with Arkajit's propagation scheme. Just within five months of starting in our group, he is making impressive progress and currently writing a draft of his results. **PRAKHAR SWARUP** who



The Huo Group at 2018 Cokerfest at Boston University (L to R): Xinyang Li, Sutirtha Chowdhury, Pengfei Huo, Prof. Bill Miller (UC Berkeley), Prof. David Coker (Boston U), Prof. John Tully (Yale), Arkajit Mandal, Sebastian Sandoval

graduated from Indian Institute of Science Education and Research joined the group as a first-year graduate student. Prakhar will bring his passion for quantum dynamics (and machine learning) to investigate excited states proton-coupled electron transfer reactions.

This year, two undergraduate students in our group, RACHEL CLUNE ('18, winner of Catherine Block and Junior Scholar Award) and ZACHARY MARSHALL-CARTER ('18) graduated. Rachel is starting her Ph.D. in theoretical chemistry at Berkeley. Zac returned to his home town in Massachusetts with plans to be a high school teacher in chemistry and biology. Former graduate student, SEBASTIAN SANDOVAL, after completing and publishing his excellent theoretical work, realized that chemistry on paper and computer did not "excite" him enough. So, he found a new place (McCamant group) that has good laser systems that can do it! We wish all of them the best for the path that they are pursuing.

The group has actively traveled and presented our new and exciting results around the world. Frank gave two talks at the APS meeting in Los Angeles, three talks at the ACS meeting in Boston, participated in the 3rd international PCET conference (and won one of the best poster prizes), and was invited to an NSF workshop at Buffalo to talk about quantum dynamics. Frank was also invited to give talks in the "quantum frontier" Telluride workshop and quantum dynamics conference in Lausanne, back to back through four flight connections from Telluride, CO to Geneva, Switzerland. With Prof. Victor Batista (Yale), Frank

also co-organized the "Cokerfest" to celebrate Prof. David Coker's 60th birthday at the Boston University (see group picture). Arkajit presented his results in a path-integral dynamics summer school at Lausanne, Switzerland, an NSF workshop at Buffalo, and at the Cokerfest, and won two best poster prizes. Arkajit, Sutirtha, and Xinyang also went to the APS meeting in Boston to present their new results. In summer, the Huo group conducted another round of "Journey to the Molecular World" summer school for local high school students in the Rochester City School District to inspire their curiosity and enthusiasm about molecular science.

In addition to the exciting research activities, Frank was also awarded an NSF career award and recognized as one of the ACS J. Phys. Chem Young Scientists. Frank also taught Computational Chemistry (CHM 469 and 470) twice in a row, before his debut of the undergraduate class in 2019, Physical Chemistry II: Statistical Mechanics, Thermodynamics, and Kinetics. We plan to keep our momentum and looking forward to another productive and wonderful year.



William D. Jones

Charles F. Houghton Professor of Chemistry

Ph.D. 1979, California Institute of Technology



RESEARCH INTERESTS

Mechanisms of reactions of transition metal organometallic compounds; activation of carbon-hydrogen, carbon-carbon, and carbon-fluorine bonds by transition metal complexes; transition metals as catalysts for the desulfurization of thiophenes in oil; electrophilic C-H activation and direct routes to aromatic amines.

CONTACT

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The **JONES** group continues our work in organometallic chemistry and catalysis. We had no first year students join the group this year, but both **ASTRID OLIVARES** and **TARAH DIBENEDETTO** have transferred in from Dan Weix's group. **HONGMEI YUAN** defended her thesis in February, and is working at RIT NTID. Bill was on sabbatical for 6 months in the spring of 2018. He received a Humboldt Senior Research Award to go to the Freie Universität of Berlin to work in the lab of Prof. Christian Müller. Christian was a postdoc with Bill in Rochester in 2000, so it was great to catch up with him and learn about phosphorus chemistry. A student in Berlin is now working on a joint project. Both Heather and Bill liked living in Berlin, and Heather even took daily German lessons for 4 months while there.

... mit dem Buddyb

Our research is examining the activation of C-H bonds in substituted hydrocarbons and the acceptorless dehydrogenation of amines and alcohols. An important recent advance has been the discovery of a new process for converting ethanol to n-butanol in a highly selective fashion, and a patent has been awarded on this discovery. Bill continues as Associate Editor for the *Journal of the American Chemical Society* for a fourteenth year, where he handled about 400 manuscripts last year. He gave talks at the Free University of Berlin, the University of Aachen, the University of Oldenburg, the University of Tübingen, the University of Würzberg, the University of Regensburg, the Technical University of Berlin, Osaka University, and Miami University. He also spoke at the International Symposium on Organometallic Chemistry



Bill with baby Charlie

Bill and Heather in Berlin-Spring 2018

in Florence and the ACS National Meeting in Boston in both the Symposium on Water Splitting & Solar Fuels, and the Jack Halpern Symposium. Bill was also the Dow Lecturer at U.C. Berkeley where he delivered two talks over a 10 day visit.

The group's scientific accomplishments have centered upon our work in amine and alcohol dehydrogenation, where we have compared iron and cobalt PNP complexes that could catalytically dehydrogenate alcohols to ketones without a hydrogen acceptor. Likewise, bicyclic amines could be dehydrogenated to quinolines without an acceptor. The reverse hydrogenations occurred readily under mild conditions. Several new nickel complexes were also examined for this reactivity. We are also extending the dehydrogenations to be carried out electrochemically. This work tied in to our recent studies of ethanol condensation to make butanol via the Guerbet process. 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. We 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).

Bill also served on the International Advisory Boards for the ICOMC and ISCHA conferences. These meetings were held during the conferences in Florence, Italy and Yokohama, Japan. The group is supported by continuing funding from the Department of Energy and the National Science Foundation.

Bill's grandson, Henry William Simson, is now 4 years old, and now has a young brother Charlie who arrived in his daughter's family in July. Both boys are doing very well, and Heather and I are delighted to see him often since they live in Rochester near Sea Breeze. Our oldest daughter Elizabeth and her husband Josh Sweet added a second dog to their family, and they live in Chili. Simon continues at iHeart Radio as Art Director while enjoying living in NYC.

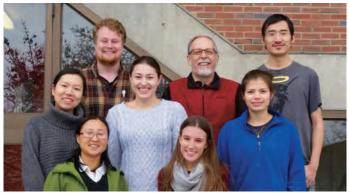


Astrid (Olivares) Parsons and Tarah DiBenedetto



Bill with former postdoc Taro Tanabe and wife Tomoko with son Kazu and daughter Lisa in Yokohama, Japan – Summer 2018





Back Row (L to R): Andy VanderWeide, Bill Jones, Ningyu Liu Middle Row (L to R): Jing Yuwen, Tarah DiBenedetto, Astrid (Olivares) Parsons Front Row (L to R): Hongmei Yuan, Kylie Ritz

Kathryn Knowles

Assistant Professor of Chemistry



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

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The Knowles group continued to grow and develop our science exploring the synthesis, electrochemistry, and photophysics of metal oxide semiconductor nanomaterials during 2018. MELISSA KOCH and JACOB SHELTON joined the group as first year Ph.D. students in January 2018. They are both working on projects using pump-probe spectroscopy to examine the excited-state dynamics of metal oxide nanomaterials. These experiments are being performed on our brand-new ultrafast laser system, which also officially joined the group in January 2018. In May, BRITTNEY BEIDELMAN joined our group as a first-year Ph.D. student from the Materials Science program to work on developing single-source molecular precursors for colloidal metal oxide nanocrystals. In the summer, we had the pleasure of hosting GARRETT HOTELING ('19), a UR undergraduate supported by a University Discover Grant, and KARLA SANCHEZ-LIEVANOS, an international REU student from Mexico. Garrett continued working with us in the fall on his senior thesis project exploring the function of copper oxide nanocrystals as catalysts for organic cross-coupling reactions. YIFENG BIAN ('19) also joined the group this fall to begin his senior thesis project developing solvothermal syntheses of nickel oxide nanocrystals.

In addition to welcoming new students to the group, we also celebrated some group members' graduations. **JORDAN ANDREWS** finished his M.S. degree and started a job as a process chemist at the Eastman Kodak Company. **JOSHUA LOMEO** ('18) and **DOMINICK SARAPPA** ('18) both successfully completed their senior thesis projects and earned B.S. degrees. Although we said good-bye to Josh, we were excited that Dom decided to stay with us for another year to complete an M.S. degree.

Research in the Knowles group reached a milestone in 2018 with the publication of the group's first two papers! Katie, Melissa, and Jacob worked together to compile a perspective article reviewing recent developments in the application of ultrafast transient absorption spectroscopy to nanostructured semiconductor thin films, which was published in the 2018 Emerging Investigators issue of the *Journal of Materials Chemistry C.* **DAVID BREWSTER** and Dom's work on elucidating the role of solvent and ligands in controlling the size and crystal structure of iron oxide nanocrystals synthesized using a solvothermal method was published in *Polyhedron* as part of a special issue honoring Bill Jones. This work also propelled David through his qualifying exam!

Katie proudly presented the group's work at several conferences over the summer, starting with a poster presentation at the 10th International Conference on Quantum Dots (QD2018) conveniently located in nearby Toronto. Katie and David both presented posters at the 2018 Gordon Research Conference on Colloidal Semiconductor Nanocrystals where Katie also served as a discussion leader. Katie then capped off her summer conference tour with an invited talk at the ACS meeting in Boston in a symposium honoring the career of Rich Eisenberg.

We are also proud to report that several members of the Knowles group received recognition for their excellent work. **MEHRIN TARIQ** earned a best poster award at the Western New York Inorganic Symposium at Cornell University where she presented her work on the surface redox chemistry of colloidal copper(I) oxide nanocrystals. Melissa was awarded a Sherman-Clarke fellowship in recognition of her outstanding academic performance as a first-year graduate student. Finally, Katie received a Valerie and Frank Furth Fund award to support her research as a promising young scientist. Nice work everyone!

In addition to all of the exciting research developments, Katie taught her graduate course, CHM 458 Spectroscopy and Kinetics, for the third time in Fall 2018 and also taught CHM 232 Molecular Spectroscopy for the first time in Spring 2018. This upper level lab course, which Katie remembers fondly from her time as an undergraduate at UR, ran relatively smoothly with a rookie instructor thanks in large part to the excellent support Katie received from her teaching assistants: David Brewster, Liwei Wang, Trevor Tumiel, and Steven Diaz. Lewis Rothberg also shared excellent advice based on his experience teaching the course in addition to completing an extensive revision of the lab manual (a.k.a. "the Green Monster") that decreased the page count from 430 to 250 in time for the Spring 2018

semester (many thanks Lewis!). Katie looks forward to continuing to develop and update CHM 232 beginning with the debut of a time-correlated single-photon counting (TCSPC) experiment in the Spring of 2019. Katie once again teamed up with David McCamant to teach an Upward Bound course focused on solar energy conversion using dye-sensitized solar cells in the summer of 2018. David Brewster, Steven Diaz, and Melissa Koch all provided valuable teaching assistance for this course.

Summer 2018 also saw the inaugural Knowles group barbecue hosted by Katie and JC at their new house in Pittsford! The Knowles group looks forward to another exciting and productive year in 2019.



The Knowles Group (L to R): Garrett Hoteling, Dominick Sarappa, Karla Sanchez-Lievanos, Melissa Koch, Kathryn Knowles, Jacob Shelton, Mehrin Tariq, Brittney Beidelman, Jordan Andrews, David Brewster

Professor of Chemistry



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; single molecule studies of protein folding structure and dynamics.

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Time for an update on **KRAUSS** group news from 2018:

Last year we said "goodbye" to several Krauss group members. ZHENTAO HOU defended her thesis, moved to the San Francisco Bay area, and promptly went back to school! Zhentao is looking to get a degree in Data Analtytics to go with her Ph.D. in carbon nanotube photophysics. Upon graduation, LEAH FRENETTE went across the pond to London, UK, where she is doing postdoctoral research at Imperial College related to using quantum dots for biological sensing. After defending her thesis AMANDA AMORI ironically decided to be a productive member of society, having taken a "real" job in Rochester working for Semrock Inc. as an applications scientist. Congrats to Amanda, Leah and Zhentao! Finally we also said goodbye to JIAJIA YIN, our visiting student from China who was with us for two years. JiaJia has synthesized CdTe quantum dots

of the highest quality, and finished an important study concerning their use in photocatalytic proton reduction with small molecule nickel catalysts.

NICOLE M. B. COGAN is writing her paper (and her final thesis chapter) on her "infamous" molecule with truly amazing photophysical properties including the ability to emit "quantum light" continuously. Yes, we still don't know what the molecule structure is – but we know it is a nice purple color! With some luck, we will get support from the DOE that will allow her to continue to search for that elusive structure. ABBY FREYER now has two papers being written related to the process of doping CdSe quantum dots with silver ions via cation exchange. Basically, Abby found that the cation exchange process produces a highly heterogeneous mixture of doped particles, undoped particles, and Ag₂Se particles, with various charges per particle. Her findings cast doubt on



the use of cation exchange as a method to dope colloidal nanoparticles reliably and reproducibly.

JENNIFER URBAN, along with a new student in the group from the Institute of Optics, WESLEY CHIANG, have conclusively shown that quantum dots can outperform organic dyes for super-resolution bioimaging purposes. Working also in Brad Nilsson's lab, they have attached peptides to the quantum dot surface that turn the nanoparticle into a fluorescent mimic of amyloid beta oligomers. They are currently looking at where these functionalized nanoparticles are going inside of live neurons. **BECKAH BURKE** has made several discoveries in the last year. In one breakthrough, she found a way to "recover" the poor photocatalytic performance of large CdSe quantum dots by adding more catalyst such that the surface of the particle is effectively saturated with catalyst. This discovery extends the useful range of solar light harvesting from the blue to the deep red wavelengths. Working in collaboration with the laboratory of Kara Bren, Beckah also found that glutathione and cobalt salts make a novel catalyst that when combined with quantum dots forms a highly efficient and robust system for photochemically reducing protons to molecular hydrogen.

SEAN O'NEILL from Materials Science made some important discoveries regarding the synthesis and photophysical characterization of SnTe quantum dots. Sean is testing whether the main absorbance feature from the quantum dots is due to a plasmon, an exciton, defects, or surface states! Given that no one really has a clue what

TREVOR TUMIEL has been busy in the time resolved room for the past year measuring the fluorescence from nominally "dark" states of carbon nanotubes. Once he completes his low temperature measurements, he will write up the first paper! MAHILET HAILEMICHAEL from Materials Science wants to get the group into lead-halide perovskites....but for now she is settling for some device engineering. Mahilet is fabricating CdSe quantum dot photocathodes that will be used for the reductive side of water splitting studies.

Finally – we want to welcome first year Chemistry student **ERIN CHRISTIANSEN** into the group! Erin is going to use electrostatic force microscopy and single particle microscopy to study defect states of long carbon nanotubes. In addition, Erin is keeping up with the recent tradition of having the nanotube project supply the group's sole interest in country music. During the summer of 2018 the group hosted another ACS Project SEED student **Rachel Kelly.** Rachel spent the summer working with the software program "Avagadro" and trying to get it to draw extended crystals. We also hosted an REU sudent from the Institute of Optics, **Malik Hamilton**, who had fun making SnTe nanocrystals with Sean and getting real cool images of them on the TEM.

Finally, don't forget that **LISA CARLSON NOGAJ** and **KATIE LEACH** put together a Facebook page for the Krauss group! We want to use it to stay in touch with current members and alums – and we want to get current updates from former Krauss group members! www.facebook.com/groups/kraussgroup



Krauss Group members (L to R): Jiajia Yin, Beckah Burke, Abby Freyer

Thomas R. Krugh

Professor of Chemistry



RESEARCH INTERESTS

Biophysical chemistry; structural analysis of biomolecules from two-dimensional NMR, fluorescence, and UV-visible spectroscopies, along with energy minimization and molecular dynamics calculations.

CONTACT

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For **TOM KRUGH**, 2018 was my transition into retirement, which began with an enjoyable, and much-appreciated, May 5th retirement dinner. Although my title changed to Professor Emeritus on July 1st, I continued as a volunteer beyond my retirement date to complete the 2018 REU (Research Experience for Undergraduates) summer program, followed by submission of the final report to the NSF (National Science Foundation). I had the pleasure of serving as director of the REU summer program from 1999 through 2018. The department plans to continue hosting UR undergraduates and international students in the years ahead.

I have been enjoying retirement, which in Fall 2018 included a September trip to the southwest to visit Zion and Bryce National Parks and a side trip to Jackson Hole, Wyoming to visit our son and his family (our granddaughters are now 8 and 10 years old. Rody (Rosemary) and I enjoy travel and have other trips planned (with some already completed in 2019).

I anticipate this as my last contribution to the Chemistry annual report, and express my thanks to all who have made my years at UR a valued experience. Meliora!









Assistant Professor of Chemistry



RESEARCH INTERESTS

The worldwide push to generate electricity from renewable sources has created a critical need to develop improved energy storage and fuel-production strategies. Research in the Matson Group focuses on using synthetic inorganic chemistry to generate multimetallic cluster complexes suitable for addressing current challenges in the fields of Energy Storage and Production.

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It was another awesome year for the Matson Group, filled with exciting changes and developments! All members of our team have continued to work hard to develop the chemistry and applications of multimetallic (polyoxovanadate) cluster complexes.

In January of 2018, we were thrilled to welcome two new group members: ALEX FERTIG (U. Cincinnati) and BRAD SCHURR (SUNY Buffalo). BRAD has been working alongside graduate student LAUREN VANGELDER, trying to understand the design principles for clusters with relevance to their application in redox flow batteries. After some hard work, he came out on top of a first author manuscript that we recently submitted to an invited issue of the Journal of Coordination Chemistry! ALEX spent most of 2018 jumping from project to project, ultimately landing on our new vacancy chemistry supporting BRITTNEY in acquiring results for our follow-up manuscript to our 2018 JACS communication. Starting this spring, Alex will be spending time working on aspects of our collaborative project with the BREN and KRAUSS laboratories, investigating electron and hole transfer phenomenon in the context of photocatalytic proton reduction (our collaborative team received funding in June from the Department of Energy to support this work!). Alex accomplished all of this while preparing for his September wedding in Columbus, Ohio to his now-wife, Alex Fertig!

In May of 2018, the Matson Laboratory welcomed postdoctoral researcher **OLAF NACHTIGALL** from the Freie University of Berlin. Olaf came to our laboratory highly recommended by prominent polyoxometalate chemists after receiving a Ph.D. with honors! His expertise on organofunctionalization of polyoxovanadate-alkoxide clusters was helpful in finishing up some outlying projects in the group. In January of 2019, Olaf will begin a new collaborative project on catalysis

between the Matson and Jones laboratories, supported by a prestigious Humboldt Fellowship.

The senior graduate students in the Matson Group (RACHEL MEYER, BRITTNEY PETEL, and LAUREN **VANGELDER**) continued their excellence polyoxovanadate synthesis in 2018 – working extremely hard to make an impact both scientifically and through outreach. The group attended multiple conferences, namely the Western New York Inorganic Symposium (LAUREN won first-prize for an amazing oral presentation!), held at Cornell University in June, and the Inorganic Discussion Weekend in Waterloo, Canada (BRITTNEY and RACHEL were both selected to give oral presentations!!). LAUREN attended both the Inorganic Chemistry GRS and GRC in June of 2018, where she made a huge splash with both an oral and poster presentation on her new redox flow battery project (in collaboration with the Cook Lab, SUNY Buffalo). The lab also took part in the Teacher's Challenge 5K to raise





The Matson Group at the Inorganic Discussion Weekend at the University of Waterloo.

money and show support for teachers in the Rochester City School District. We continue to participate in outreach and service, and particularly enjoyed the activities of *National Chemistry Week* this year, focused on planetary science!

AWARDS. The group was fortunate to be recognized with a variety of awards and honors this past year. In addition to her multiple recognitions for her performances at regional and national conferences, **LAUREN VANGELDER** was named a recipient of a Division of Inorganic Chemistry Travel Award. For her excellence throughout her time as a graduate student at the University of Rochester, Lauren was selected from a competitive pool of applicants for the *Outstanding Graduate Student Award*. We are so proud of all of her accomplishments and are excited to watch as her next steps unfold in 2019. We were all overjoyed when we received the news that **BRITTNEY PETEL** was named a recipient of the ACS Women Chemists Committee Eli Lily Travel Award, which supported her trip to the Fall

National ACS Meeting in Boston! She was also awarded the Samuel Allen and Ellen Frances Lattimore Graduate Fellowship for the second year in a row.

Undergraduate research in the Matson laboratory has continued to thrive. This Summer, we welcomed ROBERT LOVE ('19) and MICHELA MAIOLA ('20) to the team as a part of the University of Rochester REU program. In the fall semester, we increased undergraduate participation even further, welcoming RENEE NILES ('19) and JUSTINE DRAPPEAU ('21) to our research group!

ALUM: MERJEMA PURAK ('18) continued to do great things in the Matson Lab in the first half of 2018 – most notably completing her senior thesis on cross-coupling chemistry (first group paper published on this topic with graduate student **BRITTNEY PETEL**). For her excellence in undergraduate research and teaching, Merjema was named a recipient of the John McCreary Memorial Prize, the Janet Howell Clark Prize and



The Matson Group: (1st row) Michela Maiola, Brittnery Petel, Lauren VanGelder, Gabriel Santiago Martinez Alvarez; (2nd row) Robert Love, Alex Fertig, Bradley Schurr, Olaf Nachtigall, Rachel Meyer

the Carl A. Whiteman Jr. Teaching Award. Merjema was also recognized for her outstanding science and presentation skills with first-prize at the Western New York Undergraduate ACS Meeting held in Buffalo, NY. She graduated from the University of Rochester and is now a graduate student at the Massachusetts Institute of Technology. She has been busy learning all there is to know about supramolecular and polymer chemistry in the Swager Laboratory! **SAMUEL WEINSTEIN (MS, '18)** graduated with a Master's Degree in Chemistry in the spring of 2018 and is currently following his passion for high-school education in a Master's Program in the Warner School of Education. We are so proud of his accomplishments and think he will make an excellent teacher (in case you know of anyone hiring!).

We've also had the privilege of welcoming an international exchange student into the laboratory during the summer of 2018 through the international research experience for undergraduates (iREU) program at the University of Rochester. **GABRIEL MARTINEZ**, an undergraduate student from Colombia, spent the summer working with **OLAF NACHTIGALL** and **LAUREN VANGELDER** developing the syntheses of ether-derived ligands to increase the solubility of our polyoxovanadate-alkoxide clusters in organic solvent. Gabriel is now pursuing a Master's Degree in the Chemistry of Complex Systems at the University of Strausbourg.

2018 was another busy year for Ellen, filled with talking, traveling, and teaching. For her innovative teaching, Ellen was named an inaugural recipient of the Course Hero-Woodrow Wilson Fellowship for Excellence in Teaching. Ellen also had the opportunity to travel to a number of conferences in 2018, including the Fall ACS Meeting in Boston, MA and the Inorganic Gordon Research Conference held in Biddeford, Maine. She took our polyoxovanadate chemistry on the "international" circuit this year as well, participating in the International Conference on Coordination Chemistry (Sendai, Japan) and a satellite meeting for polyoxometalate chemists held at Nihon University in Tokyo, Japan. This international exposure led to her selection as the recipient of the 2018 Edith Flanigen Award for Excellence in Metal-Oxide Systems by the Humboldt University. This exciting recognition will provide Ellen with multiple trips to Berlin, Germany to cultivate collaborations with members of the metaloxide research center (CRC 1109). However, Ellen truly spent most of 2018 being exceptionally proud of the accomplishments of her research group (vide supra). She continues to feel extremely fortunate to get to work with such an outstanding group of young scientists!

Follow us on twitter (@MatsonLab) to stay up to date with the latest developments and exciting news from our group. We can't wait to see what new milestones we reach in 2019!



The Matson Group at the Teacher's Challenge 5k

electron transfer from dyes to TiO, particles. Our

new student JUAN SANDOVAL joined the group in

January 2019 after deciding he wanted to do experimental

work rather than theory. He's making rapid progress

learning how to pipette and make solutions as he

probes exciton coupling in molecular aggregates,

building on some of Mike's exciting last experiments.

Undergraduate Chem Major, ZHIHAO WU (BS, '19),

has been working with us this year and has really taken off

doing tons of solar hydrogen production work on our 16-

well hydrogen photolysis system. Chemical Engineering

major, **EKAM SINGH GILL** (ChemE BS, '19) has

also been working on that system continuing work he

began in the spring of 2018 and then handed off to

Associate Professor of Chemistry



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.

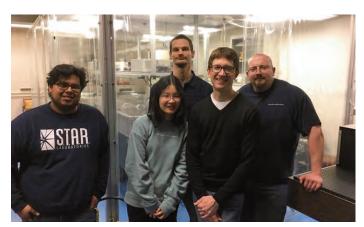
CONTACT

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The McCamant group has had a great 2018. MIKE MARK (PH.D '18) finished his thesis titled "Excited State Dynamics of Organic Chromophores Used in Solar Hydrogen Production" in August and moved on to a postdoc with Dr. Hergen Eilers at Washington State University in Spokane, WA. In Mike's absence, STEVEN DIAZ, who is now in his second year in the Ph.D. program has taken over as maestro of the Raman facility. Steven has been building up his skillset on all the lasers, so that he can take on a new project developing diffuse reflectance stimulated Raman spectroscopy. ZHI "GIGI" WU, our exchange student from Xiamen University returned home in April 2018 after working in our lab for 18 months. Gigi worked on some challenging projects including synthesis of colloidal strontium titanate nanoparticles and deciphering the electron transfer dynamics of the Eisenberg group's Pt-diimine-dithiolate dyes on TiO2. But most exciting of all, Gigi had her baby boy, Yunqi Wang (est. UR Ph.D. 2045), in August! ZAK PIONTKOWSKI, who is now in his fifth year, was our world traveler in 2018. In August, he traveled to South Korea to attend the International Conference on Raman Spectroscopy and then in September he went to Xiamen University in China for a 3-month NSF collaboration with Professor Yi Zhao. There, Zak learned new quantum dynamics methods for simulating

SABIN "SIMBA" KIM (ChemE BS, '20) over the summer.

Dave is enjoying teaching and research as usual. He was deeply humbled to receive the 2018 "College Award for Undergraduate Teaching and Research Mentorship" and to learn that so many kind students were willing to write a letter on his behalf. He was also happy to receive a "Chemmy" award and an invitation to speak from the grad students at Emory University, where our summer student Rachel Kozlowski (Summer REU 2012) is pursuing her PhD in Chemistry.



Steven Diaz, Zhi "Giqi" Wu, Zak Piontkowski, Dave, Mike Mark



Dave dining with Dr. Vivian Yam and Dr. Ching Tang

Michael Neidig

Associate Professor of Chemistry



RESEARCH INTERESTS

Physical-inorganic chemistry and catalysis: elucidation of structure and bonding in non-precious metal catalysts through inorganic spectroscopic methods; studies of reaction intermediates and mechanisms of transition metal catalysis; non-precious metal organometallics; structure, bonding and mechanism in f-element chemistry

CONTACT neidig@chem.rochester.edu

The **NEIDIG** group continues its adventures in nonprecious metal catalysis and f-element chemistry. The group currently consists of nine Ph.D. students and one postdoctoral scholar, with JOSH DEMUTH (Rollins College) joining the group in January 2018 and NIKKI BAKAS (West Chester University), MARIA CAMILA AGUILERA CUENCA (Universidad Nacional de Columbia) and ALEKSA RADOVIC (University of Belgrade) joining the group later in the year. The group also said goodbye to both DR. TESSA BAKER and DR. VALERIE FLEISCHAUER who both successfully defended their Ph.D.'s this past summer. In addition, our outstanding postdoctoral scholar DR. SAL MUÑOZ III finished up his tenure in the group this past summer and has moved on to bigger and better things at Boulder Scientific in Colorado.

The group had another highly successful research year, with publications spanning projects in iron-catalyzed reactions in organic synthesis and f-element chemistry. Of particular note was a key study determining the

role of NMP in iron cross-coupling (Angew. Chem. Int. Ed. 2018), a critical advance in our understanding of simple salt catalyzed cross-coupling. Not to be outdone, STEPHANIE CARPENTER published an exhaustive study of homoleptic iron-phenyl species involved in cross-coupling (Chem. Sci. 2018) while JEFF SEARS and Sal extended our studies to some unbelievable ironethyl complexes (Angew. Chem. Int. Ed. 2019). Valerie, Pete and Sal published our first investigation of iron-NHC cross coupling, establishing the key reactive iron species in a cool alkyl-alkyl cross-coupling system (Chem. Sci. 2018). The group has also continued to spread the word on the utility of physical inorganic methods in evaluating iron catalyzed cross-coupling, including a critical perspective in J. Am. Chem. Soc. in 2018 by Jeff and Pete and an Acc. Chem. Res. article in 2019 to which everyone contributed, which summarizes our key contributions to the field over the past five years. Beyond iron, the group continues its foray in electronic structure studies of actinide complexes, publishing our second uranium MCD investigation





Tessa Baker and Valerie Fleischauer celebrating after their PhD defense



Inorganic discussion weekend (L to R): Jeffrey Sears, Theresa Iannuzzi, Nikki Wolford, Stephanie Carpenter



The Neidig Group: (1st row) Nikki Wolford, Peter Neate, Stephanie Carpenter, Nikki Bakas, Theresa lannuzzi, Maria Camila Aguilera-Cuenca; (2nd row) Joshua DeMuth, Dan Curran, Michael Neidig, Jeffrey Sears

as part of a collaborative project with Los Alamos National Laboratory. We have continued (or have started) exciting collaborations in f-element chemistry over the past year with groups at the University of Edinburgh, Trinity College Dublin, Florida State University, Purdue University and Los Alamos National Laboratory. As always, the group's research accomplishments are all down to the outstanding student and postdoctoral researchers in the group, many of which were individually honored this past year. THERESA IANNUZZI received a prestigious Elon Huntington Hooker fellowship from the University of Rochester. Theresa and Stephanie also received travel awards to support the presentation of their work at the ACS National Meeting in New Orleans Spring 2018. Last, but certainly not least, NIKKI WOLFORD was also recognized with the 1st place poster award at this past year's Inorganic Discussion Weekend meeting held at the University of Waterloo.

The group also once again hosted students from Monroe Community College (CHRISTOPHER THAINE) and a local high school (PATIENCE GIRIGIRI) for summer research experiences. Patience's work was published as well – a great accomplishment for a secondary school student! As has become tradition, many members of the group ventured north of the border in November for the Inorganic Discussion Weekend meeting at the University of Waterloo. Theresa, Stephanie, Jeff and Nikki all presented their work. Furthermore, Theresa and Stephanie also both attended the ACS National Meeting in New Orleans in Spring 2018. Mike had several long distance trips again this past year to spread the word on the group's most recent chemistry, including talks at the ISHC (Amsterdam), ICOMC (Florence, Italy) and NoNoMeCat (Rostock, Germany) meetings. Additional trips included university seminars in the states of Wisconsin, Texas and Florida amongst others. Moving forward, we anticipate another exciting year of research in non-precious metal catalysis and f-element chemistry at Rochester.

Associate Professor of Chemistry



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 **NILSSON** group continued to evolve and progress in 2018. The group published five peer-reviewed publications, taught classes as instructor or teaching assistants, and had a new research grant funded by the American Heart Association. Brad and former graduate student, **TODD DORAN** (University of Minnesota, Department of Medicinal Chemistry) edited a volume of Methods in Molecular Biology that was published in 2018. Graduate students are reaching significant milestones, with several finishing up their Ph.D. work and preparing for their thesis defenses.

DANIELLE (RAYMOND) RIEGLE completed her Ph.D. thesis research during the summer of 2018 and accepted a position at Bausch and Lomb. She returned to defend her Ph.D. thesis, "Multicomponent Supramolecular Peptide Biomaterials", in February 2019. In addition to completing her Ph.D. thesis, Danielle also coauthored a monster 62-page review paper, Multicomponent Peptide Assemblies (Chem. Soc. Rev. 2018, 47, 3659-3720), that was a massive undertaking. Her work was instrumental in moving our research program toward applications of our novel biomaterials. For example, she initiated a new collaboration for our group (with Dr. Takahiro Takano, UR Medical Center) in the application of our gels for the sustained and localized delivery of pain medications and this work has been recently published (ACS Applied Bio Materials 2019, 2, 10.1021/acsabm.9b00125). This work demonstrated the sustained relief of pain due to inflammation in mice for 2 weeks from a single injection of a hydrogel loaded with an anti-inflammatory drug. We're excited by the potential of this exciting research! Danielle has been incredibly successful in her position at Bausch and Lomb, having been recently promoted after less than a year at the company. We congratulate her on the completion of her Ph.D. studies and we're confident in her continued success.

JADE (WELCH) RUSSELL has continued her work on the mechanism of action for the peptide-based in vivo delivery of therapeutic oligonucleotides in collaboration with Professors David Dean and Arshad Rahman in the University of Rochester Medical Center. In June of last year, Jade married her fiancé Blake Russell. Many of the group members attended her wedding and both Jen and Danielle were bridesmaids. Jade is nearing the completion of her Ph.D. studies and will defend her Ph.D. thesis in the near future. Jade has recently received (and accepted) a job offer from Bausch and Lomb and will start this position shortly!

JEN URBAN, a member of both the Nilsson and Krauss groups (in collaboration with **Dr. Handy Gelbard** in the University of Rochester Medical Center), is also nearing the end of her time at the University of Rochester. Her project focused on the development of quantum dots for super resolution biological imaging of neurons is nearly complete and thesis-ready after years of heroic pioneering work. She plans to defend her Ph.D. thesis in June 2019. In addition to her great work in the lab, Jen has also been quite well travelled in the last year. She



Danielle,, Jen, Jade, Brittany and Elena at Jade's wedding

presented the results of her work at the Single Molecule Biophysics Meeting (Aspen Center for Physics) in Aspen, CO in early 2019 (the second time she's attended this conference). In addition to her thesis work, Jen has also initiated a new collaborative project (with Marc Halterman, Craig Morrell, and Scott Cameron of the University of Rochester Medical Center) using functionalized magnetic nanoparticles to model stroke in mice. This project has recently been funded by the American Heart Association and Jen has been critical in the early work. She is also currently interviewing for post-graduate positions and we're excited to see where she lands.

BRITTANY ABRAHAM continues to study the selfassembly of low molecular weight amino acid derivatives toward the design of novel supramolecular hydrogels for drug delivery and tissue engineering. She is excited to be fully focused on her research now that she has finished her coursework and has contributed to our recently published work on the development of hydrogels for drug delivery (ACS Applied Bio Materials 2019, 2, 10.1021/acsabm.9b00125). Outside of the lab, Brittany helped Brad develop a new curriculum for "The Science of Slime," our week-long summer Upward Bound course with the Kearns Center for high school students from the Rochester City School District. The handson experiments, ranging from making slime to creating edible hydrogels, were a hit with the 24 students enrolled last summer. Brittany also did science demonstrations about the chemistry of the solar system at some of the city schools as part of the department's National Chemistry Week events. Lastly, Brittany started working with the Kearns Center to lead a study group for organic chemistry students, and hopes to continue this excellent experience throughout her graduate career to hone her teaching skills.

ELENA QUIGLEY has spent the past year developing her project in structural investigation of self-assembled biomaterials. She is seeking to correlate structure to the physical properties of emergent hydrogels in order to develop rational design strategies for next-generation biomaterials. In pursuit of this goal, she authored and submitted a proposal to the National High Field Magnetic Laboratory at Florida State, and is working under the guidance of **Dr. Riqiang Fu** to interrogate these structures by solid-state NMR. Elena has also been pursuing her passion for teaching, both in the classroom and the laboratory. In the past year she has maintained a position as an Organic Chemistry Study Group Leader



Brad and Trista at Jim Farrar's retirement party

at the Kearns Center for Learning and Diversity. She also participated in the Upward Bound Summer program and National Chemistry Week, to help spark scientific interest in high school students from the local area districts. Elena also presented her research at the ACS Spring National Meeting 2019 in Orlando, both at the Sci-Mix poster session and in her selected symposium: LGBTQ+ Graduate Students and Postdocs, for which she received a travel award. We're very excited about her early work.

The Nilsson group welcomed two new students in the fall of 2018. MELISSA JAGROSSE grew up in West Haven, CT and received a BS in Biology and Chemistry from Southern Connecticut State University. During her undergraduate career she actively participated in research projects in the fields of mammalogy, paleontology, and organic synthesis. Melissa's current research involves the development of macrocyclic peptides for the delivery of siRNA to cells. This work is picking up where Jade is leaving off. In addition to her graduate studies, Melissa is a dedicated CrossFit athlete, training at CrossFit RSG 6 days per week. **FRANCINE YANCHIK**, originally from Ft. Lauderdale, FL, spent the majority of her life in Syracuse, NY. She received her BS in Biochemistry with a minor in History from Le Moyne College in 2018. She now studies peptides for aggregation of blood platelets along with the self-assembly of amyloid-like peptides in the Nilsson group. Both Melissa and Francine are off to a great start in the research lab.

The Nilsson group has continued to benefit from the work of excellent undergraduate research students. **ETHAN TORIKI**, a University of Rochester student in biochemistry, spent summer 2018 conducting research in the Nilsson group, and coauthored a recently published

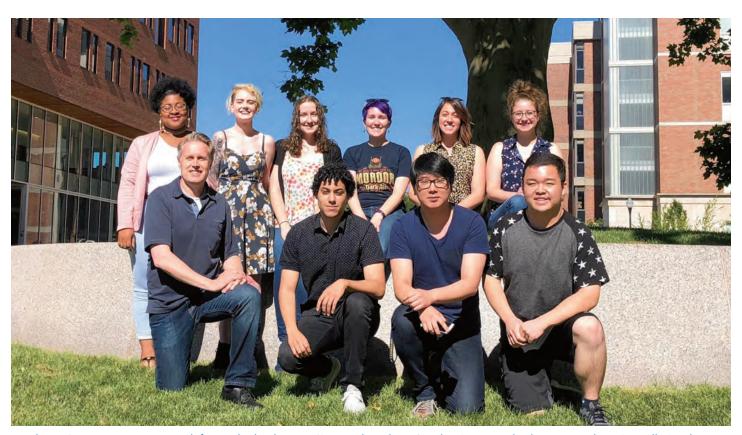


Danielle, Jade and Jen

manuscript that he contributed to (ACS Applied Bio Materials 2019, 2, 10.1021/acsabm.9b00125). He is nearing completion of work on a second manuscript based on his mentored projects (with Brittany Abraham). N'DEA TUCKER, another University of Rochester undergraduate, also worked in the Nilsson lab during the summer of 2018. She worked with Ethan on a study regarding the comparative rates of release of molecules from hydrogels for drug delivery applications. Her work was supported by a research fellowship from the McNair Research Program. Ethan and N'Dea were both mentored by Brittany Abraham. MATT WATROUS also

contributed to these projects. **JOHNATHAN NEGRON VELLALBA** (Universidad Metropolitana, Puerto Rico) was an REU participant during summer 2018 and worked with Elena Quigley on the synthesis of self-assembling peptides containing modified lysine residues. Finally, **JISOO WOO** worked with Jen Urban on the synthesis and analysis of self-assembling amyloid-beta derivatives. Overall, this has been an outstanding collection of talented undergraduate research students!

In addition to working with these outstanding researchers, Brad continued to serve as chair of the Harrison Howe Award Committee (Rochester Section of the American Chemical Society), Treasurer of the American Peptide Society, and Chair of the Travel Grant Committee for the 2019 American Peptide Symposium. He completed his term as Chair of the Department of Chemistry Graduate Studies Committee and handed those responsibilities over to Joe Dinnocenzo in the fall of 2018. He inherited the first semester Organic Chemistry course (CHM 203) in the Fall 2018 semester and taught that course for the first time since joining the department. The challenges of managing nearly 400 anxious organic chemistry students was a major undertaking, one that he's eager to refine in the coming year! Life is busy and life is good! We're excited for a new year of challenges.



Nilsson Group June 2018. From left to right; back row: N'Dea Tucker, Elena Quigley, Brittany Abraham, Jen Urban, Danielle Riegle, Jade Welch. Front row: Brad Nilsson, Johnathan Negron Villalba, Jisoo Woo, Ethan Toriki.

Lewis J. Rothberg

Professor of Chemistry



RESEARCH INTERESTS

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

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LEWIS ROTHBERG'S group continues to investigate conjugated polymer photophysics and has expanded to studies of water soluble fluorescent polymers that may be suitable for biological imaging. LIWEI WANG is making very good progress studying the single chain spectroscopy of new systems while also having substantially upgraded the confocal microscope's capabilities. She has gracefully taken on many organizational and mentorship roles in our small group. Meanwhile, ZIYANG YE is working hard to unravel the mysteries of conjugated polyelectrolytes in solution for his MS research and is well on the way to publishing his results. The group has had a very strong cadre of undergraduate researchers this year. UR students TIANHAO YU (phosphor hosts made by Molecular Glasses) and JIEYU HE (magnetic field effects on delayed luminescence in conjugated polymers) were joined by ALEKSA RADOVIC (thermally activated delayed luminescence, TADF) from Serbia through the international REU program. Aleksa is now matriculated into the Neidig group as a graduate student. In a strange twist of fate, Lewis met Dr. Mitch Nelson who had published very interesting theory concerning TADF and it turned out that Aleksa has been using his theory. The relationship with Dr. Nelson has evolved to bring new ideas into the group that may trigger a wave of interesting new research. Their efforts have been supplemented by an evolving collaboration with Profs. Linda Peteanu (Carnegie Mellon) and Eric Fossum (Wright State) on new blue TADF emitters. XIN HUANG (Materials Science MS) graduated in the Spring and went to begin a PhD at UCLA but made such good progress developing reflective interferometric sensing that Lewis decided to take on a joint PhD student with Alex Shestopalov, FAKHRADDIN DOURBASH AKBARI. It is gratifying to see that project going so well after so many years of struggle. While the group is very small, there is lots of activity and our colleagues DR. RALPH YOUNG and DR. AL MARCHETTI (now recovered from poor

health in late 2017) continue to do their own research and mentor students. We have also merged our group meetings with those of the McCamant group which has made for lots of interesting educational opportunities and a sense of critical mass.

Lewis was formally on sabbatical leave in 2018 and spent a substantial portion of his time researching and writing materials pertaining to environmental chemistry. Lewis' long term goals under that umbrella are to write a book for the public on the role and importance of Chemistry as it pertains to sustainability issues and also to dramatically change the content in General Chemistry to make its relevance to our future clearer to first year students. Lewis missed teaching and looks forward to returning to the classroom reinvigorated with new material and new ideas while he continues to work on the book.

In January, Lewis attended the National Council for Science and the Environment annual meeting in Washington and also received formal training in science communication for the public and policy makers. While in Washington, he initiated a joint project with NOAA to publicize the importance of NOAA's Ocean Monitoring program (ARGO). It was an extremely stimulating year and an exciting inflection point in Lewis' career where his focus is shifting towards the larger role of science in the society. Lewis also had an inspirational trip to the sustainability institute at Arizona State University where many of the pieces of the vision behind the sabbatical are being put into practice. In addition to those types of "off road" sabbatical activities, Lewis gave an invited talk at the summer ACS meeting on Liwei Wang's and Ben Martin's work. Also, Lewis was honored to be the Closs Lecturer, elected by the University of Chicago graduate students to present our group's work at their seminar. Gerhard Closs is something of an idol to Lewis who has used excerpts from Closs' work in teaching Chemistry 252 (advanced thermodynamics and kinetics). It was a very happy occasion that also enabled Lewis to see former group member Chris Melnychuk who is thriving in his PhD research. The added twist of Chicago being **ESTHER CONWELL'S** PhD alma mater was another nuance that gave the trip special meaning. Lewis continues to direct the Materials Science program at the University along with outstanding support and initiative from **GINA EAGAN**. It will probably be his last year as director and he is both relieved and gratified to have left the program in good shape and brought forward some educational and team-building initiatives that are appreciated by the students.

A very special moment this year was the awarding of the first **ESTHER CONWELL** graduate fellowship to **ZAK PIONTKOWSKI** from the McCamant group. Esther would have been so proud of Zak whose curiosity, talent and drive have led him to do both extensive theoretical and challenging experimental work for his thesis. Lewis and Shelby are very appreciative of those who joined us in making this possible. Another memorable event was

Jim Farrar's retirement. The affection for Jim that his students and colleagues feel is palpable, a feeling Lewis shares. Not a course goes by when Lewis does not think about the many contributions made to his notes and knowledge by Jim and by John Muenter. Shelby continues the fast-paced life of a Chief Technical Officer and has helped to move her company Mosaic Microsystems forward into their own manufacturing space. It's exciting to watch. Charles is a junior at Pittsford Mendon High School beginning to think about college while enjoying sports, debate and history. Vivian has moved to the Harley School and is blossoming both socially and academically. Her interests span the spectrum from creative writing to algebra to composing music and she seems able to find joy in almost everything she does. Lewis has taken an active role in the management of his synagogue this year. He is looking forward to teaching General Chemistry once again leading up to a summer backpacking trip with his friends from UR class of '77, a throwback to the cross-country camping trip they took over 40 years ago!



(L to R): Tianhao Yu (ChE); Liwei Wang, Xin Huang (MatSci), Lewis Rothberg, Yongli Lu, Al Marchetti, Raj Chakraborty

Wolf-Udo Schröder

Professor of Chemistry

Ph.D. 1971, University of 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

schroeder@chem.rochester.edu

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 program investigating reactions between light nuclei. In a first nuclear experiment, the group has utilized the intense neutron flux (~1014 per 'shot') produced at the LLE-Omega facility in laser-induced inertial confinement fusion events. Here, neutron-induced breakup of deuterium was detected and analyzed.

A new experimental platform LIANS (Laser Ion Acceleration for Nuclear Science) has been installed and used to produce an energetic (MeV) deuteron beam. A first proof-of-principle experiment, a (d,n) stripping reaction on ⁹Be, turned out results consistent with known data measured in very different, accelerator-

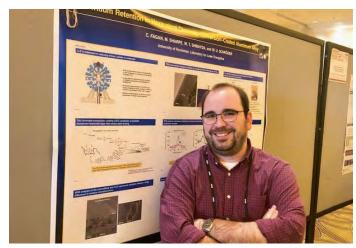
based experiments. This is considered an important milestone towards producing a tritium beam by the same mechanism. A vacuum evaporation setup has been designed and constructed to produce titanium targets loaded with select isotopes of hydrogen. Grad student Arnold Schwemmlein succeeded in demonstrating the method with shots at two powerful laser systems at LLE, the MTW and the OMEGA/EP facilities. Experience gathered in these precursor measurements will be instrumental in the development of the LIANS platform for triton beams. While the focus of the MTW study was optimization of target characteristics, such as evaporated thickness, with a low energy laser system, the OMEGA-EP study examined the scalability to a high energy system and the use of established nuclear diagnostics. Udo outlined the program at the Int. Direct- Drive ICF and HED Workshop held at the



Cody Fagan, Dan Bassler, and former grad student Matt Sharpe

LLE and made remarks at the August-2018 Workshop on Nuclear Processes in Dense Plasmas at Livermore National Laboratory. Arnold spoke about the program at the Oak Ridge tritium meeting.

Grad students Cody Fagan and Dan Bassler continued work on our experimental radio-chemical study of tritium transport in metals. They have recently focused on the importance of surface properties when characterizing tritium uptake in metals. Designer surfaces, such as atomic layer deposited Al₂O₃ on stainless steel have been exposed and compared to samples that have no surface modifications. Preliminary data suggests that precise control of surface characteristics, such as porosity, film density, and chemical surface states, is necessary. The eventual task is to understand and produce surface located barriers on metals that suppress tritium uptake by the metal lattice. Using a variety of surface modification techniques, resulting "designer" surfaces were characterized with a set of diagnostic tools available at the URNano systems center.



Cody Fagan at poster session

Cody and Dan have presented results of their work at the Oak Ridge and Albuquerque workshops and tritium focus group meetings. Cody has also lectured at the Orlando TOFE meeting and is scheduled to present the latest aluminum coating data at the upcoming Int. Conf. on Tritium Science and Technology in Busan/South Korea.



Udo and his wife Chojy at Jim Farrar's retirement party.

Douglas H. Turner

Professor of Chemistry



RESEARCH INTERESTS

Biophysical chemistry: nucleic acid structure and function, prediction of RNA structure from sequence, RNA folding, and design of therapeutics that target influenza RNA.

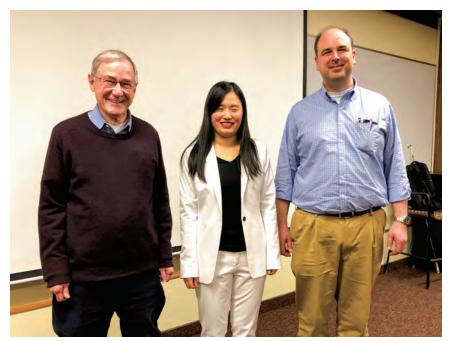
CONTACTdouglas.turner@rochester.edu

Doug continues his transition to computation as a path to expanded understanding of RNA physical chemistry. KYLE BERGER (Biophysics) and ANDY KAUFFMANN (Chemistry) defended their Ph.D. theses. Kyle studied the thermodynamics and NMR structures of several RNA duplexes with 2 by 2 nucleotide internal loops closed by GU pairs. The thermodynamics were published in collaboration with DAVE MATHEWS (PH.D. '01, M.D. '03), SUSAN SCHROEDER (PH.D. '02), BRENT ZNOSKO (PH.D. '04), SCOTT KENNEDY, and HONGYING SUN, a graduate student in the Mathews' group. The NMR is being published with Scott in Biochemistry and is now on the journal's Kyle discovered unexpected sequence website. dependence of stability and structure. The results will help improve predictions of secondary and 3D structure and serve as benchmarks for testing force fields used for computations. Kyle accepted a postdoc with David MacLean in the Department of Pharmacology and Physiology in UR's School of Medicine and Dentistry.

Andy started a position as Assistant Professor of Chemistry at Truman State University in Missouri. He returned to Rochester to defend his thesis, which focuses on structures for two RNA sequences from influenza A. In order to start teaching in the Fall, additional NMR experiments on an influenza A motif will be written up in the summer of 2019.

While Kyle and Andy were finishing their theses, Doug, Scott, and **JIANBO ZHAO** were integrating into the Mathews' group. One gratifying result from





Doug, Hongying Sun, and her advisor David Mathews

combining molecular dynamics (MD) simulations with NMR was publication of a paper reporting the unusual minor conformation of the internal loop in the duplex, (GACGAGUGUCA)₂. While GU and AG pairs formed, neither had the expected hydrogen bonding. This structure complements the novel major structure (published in 2012) where neither GU nor AG pairs form. Together, the results provide a stringent test of whether force fields can approximate hydrogen bonding, stacking, hydration, and other interactions well enough to accurately predict 3D structures of RNA without requiring experiments. The Mathews' group also used optical melting data from Kyle and **JON CHEN (PH.D.**

'15) for testing a new approach used for analyzing such data.

To isolate stacking from base to base hydrogen bonding, the group has used NMR and MD to study single stranded tetranucleotides. Jianbo partnering with Scott Dave Mathews to extend this research to RNA and DNA with the sequence, UCAAUC. The MD simulation results differ markedly from those on CAAU and also between RNA and DNA. Jianbo's research won her an Elon Huntington Hooker fellowship in the University-wide competition. Detailed interpretation of NMR for single strands is complicated because there is an ensemble of structures rather than a single structure. With considerable help from Scott, groups in Trieste and Copenhagen published an approach to combine NMR and MD to define key conformational states in an ensemble.

Doug enjoys celebrating the achievements of former members of the group. Susan Schroeder was appointed to the editorial boards of Science Advances and the Biophysical Journal. **MATT DISNEY (PH.D. '02)** won the prestigious Sackler Prize in Chemistry from Tel Aviv University. Additionally, his company, Expansion Therapeutics, received commitments of

over \$50 million in startup funding. RNA is emerging as a target for therapeutics. Part of the enthusiasm for this paradigm arises from the success of the Ionis/Biogen oligonucleotide therapeutic, SPINRAZA, that binds to an abnormal mRNA and allows more normal muscle development in children. SPINRAZA brought at least \$1 billion worth of happiness to both families and stockholders last year. **SUE FREIER (POSTDOC, '80-'86)** was one of the first 30 employees of Ionis, and became a Vice President. It is exciting to see a dream of the RNA community realized after more than three decades and to anticipate further advances, including from Expansion Therapeutics.



Doug and Joanna at Jim Farrar's party

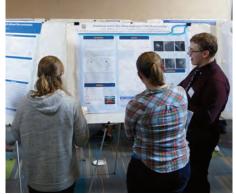
Senior Poster Session



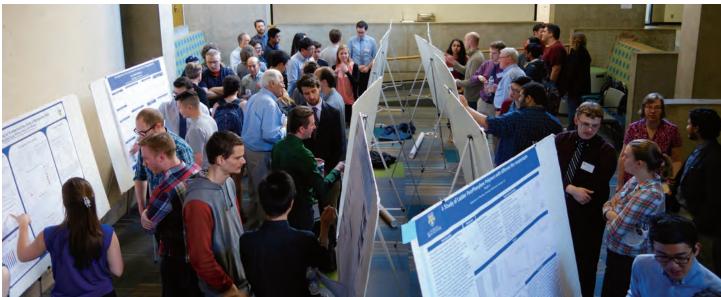
Class of 2018 Senior Thesis Poster Session

1st row: Yashika Sharma, Merjema Purak, Claire Dickerson, Rachel Clune, Yongli Lu; 2nd row: Ilan Goldberg, Dominick Sarappa, Joshua Lomeo, Chen Chen, Alex Callahan, Zachary Marshall - Carter, Caleb Whittier, Noah Sims









Commencement

Bachelors and Masters Degrees Awarded in Chemistry

2018 BACHELOR OF SCIENCE

2018 BACHELOR OF ARTS

Austin Bailey^{2**}
Alex Callahan³
Hayden Carder^{3†}
Chen Chen^{3†}
Claire Dickerson¹
Ilan Goldberg
Joshua Lomeo

Yongli Lu³
Zachary MarshallCarter¹
Merjema Purak^{3†}
Dominick Sarappa
Noah Sims

Nickolas Andreacchi Colleen Arnold² Ursula Bertram Dosung Byun Rachel Clune^{3†} Alyssa Flaschner² Michael Gannon² Alisa Groom

Caitlyn Normanı

Andrew Olsen
Carrighan Perry
Ryan Rosen
Stefan Sarkovich¹
Yashika Sharma¹
Katherine St. George
Caleb Whittier
Ryan Wong¹

¹Distinction ²High Distinction ³Highest Distinction [†]Phi Beta Kappa *Take 5 Scholar (beginning) **Take 5 Scholar/KEY Program (finishing)



Class of 2018 Bachelor's Degree Recipients

2018 MASTER OF SCIENCE

Shukree Abdul-Rashed Jose Alvarez-Hernandez Jordan Andrews Daniel Bassler David Brewster Daniel Curran Arkajit Mandal Leopoldo Mejia-Restrepo Juan Sandoval Ryan Shannon

Jesse Stroka
Andrew Vander Weide
Liwei Wang
Samuel Weinstein
Nikki Wolford























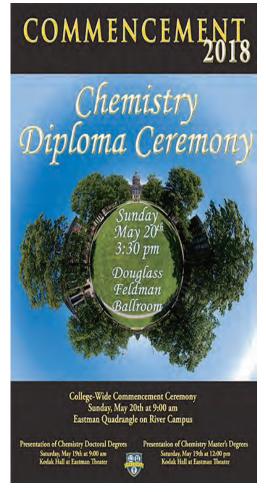












Doctoral Degrees Awarded in Chemistry

Ph.D. Degrees Conferred on March 9, 2018

Leah Frenette

Colloidal Quantum Dot Synthesis Mechanistic Studies, and Applications in Photocatalysis Advisor: Todd D. Krauss

Ph.D. Degrees Conferred on May 19, 2018

Amanda Amori

Photophysics of Single-Walled Carbon Nanotubes and Their Applications Advisor: Todd D. Krauss

Zhentao Hou

Photophysical Properties of Single-Walled Carbon Nanotubes

Advisor: Todd D. Krauss

Hongmei Yuan

Synthesis and Characterization of Group VIII & IX Transition Metal complexes and Their Application in C-H Bonds Activation and Hydrogen Transformation

Advisor: William D. Jones

Ph.D. Degrees Conferred on August 31, 2018

Yixing Guo

Cobalt Metallopeptide for Multi Proton, Multi Electron Reactions Advisor: Kara L. Bren Ph.D. Degrees Conferred on October 5, 2018

Tessa Baker

Insight into Iron Chemistry in nature and Catalysis through Electronic Structure, Bonding and mechanism Studies

Advisor: Michael L. Neidig

Andrew Owens

Strategies for the Evolution of macrocyclic Peptide Inhibitors of Protein-Protein Interactions

Advisor: Rudi Fasan

Ph.D. Degrees Conferred on December 31, 2018

Michael Mark

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

Kyle Rugg

I. 2nd Generation Total Synthesis of (-)-Nakadomarin II. Studies Toward the Total Synthesis of (-)-Apoptolidin A Advisor: Robert K. Boeckman, Jr.

Eric Stoutenburg

Studies toward the Total Synthesis of Tetrapetalone A
Advisor: Alison J. Frontier

Jing Yuwen

Activation of O-H/N-H Bonds by Rhodium Complex

Advisor: William D. Jones



Student Awards

DEPARTMENT AWARDS

Dr. E. W. and Maude V. Flagg Award

2018: Hayden Carder



Established in 1982 as an endowed fund by Dr. John J. Flagg ('36), this award recognizes outstanding performance and promise in chemistry by a graduating senior. A faculty committee appointed by the Chair of the Department of Chemistry selects the recipient.

ACS Rochester Section Award

2018: Rachel Clune

This award is given to a senior with an outstanding academic record and consists of a cash prize, recognition during the ACS Annual Rochester Section Undergraduate Research



Symposium, and the inclusion of the awardee's name on a plaque displayed in the department.

ACS Inorganic Chemistry Award

2018: Alex Callahan

This award is given to a student who is selected by the faculty on the basis of outstanding academic achievement in inorganic chemistry.



John McCreary Memorial Prize

2018: Merjema Purak



The John McCreary Memorial Fund was established in 1985 in tribute to the high academic and scientific standards and the personal dedication of John James McCreary. McCreary received his bachelor of science degree in chemistry with high distinction from the University of Rochester in 1975.

ACS Organic Chemistry Award

2018: Chen Chen

This award is given to a student who is selected by the faculty on the basis of outstanding academic achievement in organic chemistry.



ACS Physical Chemistry Award

2018: Yongli Lu

This award is intended to encourage student interest in physical chemistry and to recognize students who display an aptitude for a career in the field.



Chemistry Department Award

2018: Colleen Arnold, Alyssa Flaschner, Michael Gannon, Yashika Sharma









The Chemistry Department Award is given to seniors in recognition of outstanding scholarship in the study of chemistry. The award consists of a certificate and cash prize.

TEACHING AWARDS

Carl A. Whiteman, Jr. Teaching Award

2018: Hayden Carder, Rachel Clune, Michael Gannon, Merjema Purak, Dominick Sarappa







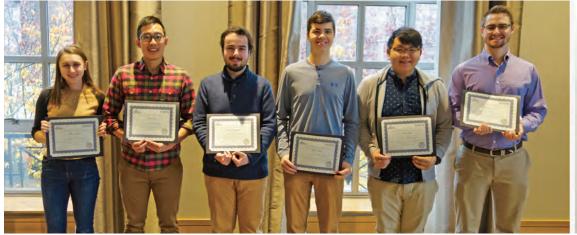




The Carl A. Whiteman, Jr. Teaching Award recognizes exemplary teaching by an undergraduate student in the Department of Chemistry. Carl Whiteman graduated from the University of Rochester in 1950 (BS, Physics) and worked continuously in the department until his retirement in 1986. His enthusiasm and dedication to laboratory teaching made him a legendary figure among undergraduate chemistry majors. Whiteman continued his association with the department until his death in 2007. This honor recognizes his teaching experience, as well as that of the recipients.

Junior Scholar Award for Juniors

2018: Allison Stanko, Nicholas Lim, Robert Scappaticci, Marco Caiola, Andrew Lee, Patrick Forrestel, and Ian Brodka





This award recognizes undergraduate students who, in their junior year, showed outstanding accomplishment and promise for a professional career in chemistry.

COLLEGE AWARDS

Janet Howell Clark Prize

2018: Rachel Clune, Merjema Purak





The Janet Howell Clark Prize is awarded annually to the senior woman who has shown the greatest promise in creative work in either astronomy, biology, chemistry, or physics, and who has shown outstanding versatility in the mastery of allied fields. Selection is based on recommendations by the respective departments, which are evaluated by a committee appointed by the Dean of the College.

PHI BETA KAPPA

2018: Hayden Carder, Chen Chen, Rachel Clune, & Merjema Purak



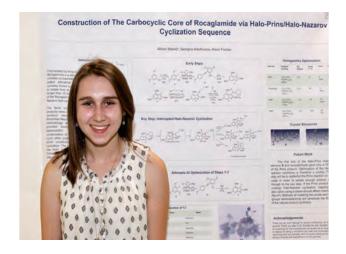






Catherine Block Memorial Fund Prize

2018: Allison Stanko



The Catherine Block Memorial Fund Prize, established in memory of Catherine Block, an exceptional chemistry student here at the University, is awarded each year to a woman in the junior class in recognition of her outstanding ability and achievement in the field of science. Selection is based on recommendations by the respective departments, which are evaluated by a committee appointed by the Dean of the College.



Celebrating at the Departmental Fall Awards Gathering

ENDOWED DEPARTMENT FELLOWSHIPS

Robert & Marian Flaherty DeRight Fellowship

2018: Sutirtha Chowdhury, Jeffrey Sears





This fellowship was established in 1984 by Mrs. Marion DeRight as a memorial to her husband Robert. Dr. and Mrs. DeRight received their bachelor's degrees from the University of Rochester in 1931, in chemistry and romance languages, respectively. Robert continued his graduate studies at UR and received his Ph.D. in 1935 with advisor Professor Edwin Wiig in physical chemistry. Dr. DeRight was a lifelong valued member of the American Chemical Society, and both he and his wife were active in alumni affairs at the University of Rochester. It provides a graduate fellowship in the Department of Chemistry for a term of one year.

Moses Passer Fellowship

2018: Stephanie Carpenter

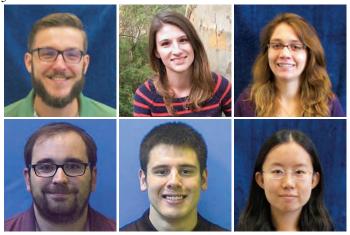
This endowed fellowship fund was established by Mrs. Dorothy Rosenberg-Passer in 2009 in memory of her husband, Dr. Moses Passer, who received his bachelor of science degree in chemistry from the University of Rochester



in 1945 and his doctorate in organic chemistry from Cornell in 1948. After a distinguished career as professor of chemistry at the University of Minnesota Duluth, Dr. Passer became an executive at the American Chemical Society in Washington, DC, and served as director of education at the ACS for more than two decades.

Elon Huntington Hooker Fellowship

2018: Georgios Alachouzos, Rebeckah Burke, Theresa Iannuzzi, Cody Fagan, Eric Moore, Jianbo Zhao



The Elon Huntington Hooker Fellowships are awarded from a gift from Mrs. Elon Huntington Hooker in memory of her husband, Elon H. Hooker, a graduate and, for many years, a trustee of the University. These fellowships are awarded in various fields of science, especially chemistry.

Samuel A. & Ellen F. Lattimore Fellowship

2018: Brittney Petel, Viktoria Steck





This endowed fellowship honors Professor Samuel A. Lattimore and his wife, benefactors of the University of Rochester from its earliest days. The fellowship was established by a gift from the estate of Eleanor Larrebee Lattimore. Professor Lattimore was associated with the University of Rochester for more than 40 years and began his career at Rochester teaching chemistry, being his chief concern, but also geology, zoology, and physics. He was chair of the Department of Chemistry from 1867-1908. The fellowship is designed to support outstanding graduate students in the Department of Chemistry and gives special consideration to women applicants.

Robert L. and Mary L. Sproull Fellowship

2016-2019: Jesse Stroka



2018-2020: Brittany Abraham



The Sproull Fellowship is a prestigious award given by the University of Rochester to twelve incoming doctoral degree students. This 3-year fellowship honors Robert L. Sproull, a distinguished physicist and the University's seventh president, and reflects his commitment to intellectual excellence. The fellowship candidates are nominated by their Ph.D. programs and evaluated by a committee of faculty members. The final selection is made by the University Dean of Graduate Studies.

Arnold Weissberger Fellowship

2018: Jose Alvarez-Hernandez, Arkajit Mandal, Leopoldo Mejia Restropo, Juan Sandoval









The purpose of the Weissberger Fellowship in Chemistry is to reward and encourage outstanding promise for productive scientific careers by advanced Ph.D. students. Each Fellow receives a substantial supplement for basic support and funds to travel to a major scientific meeting to report the results of his research. The fellowship is awarded on the basis of outstanding research achievement and potential for continued growth, ideals which Arnold Weissberger exemplified during his lifetime and which he recognized and encouraged in others.

Esther M. Conwell Fellowship

2018: Zachary Piontkowski

Dr. Esther Conwell, born in 1922, was a female pioneer in Chemistry and Physics. Created to honor her scientific accomplishments, this fellowship provides support for a graduate student in Chemistry



who shows exceptional promise as a researcher. Conwell was recognized as one of Discover magazine's Top 50 Women of Science in 2002 and was awarded the National Medal of Science by President Barack Obama in 2010. A pioneer in semiconductor research that revolutionized modern computers, her expertise earned her the rare honor of being the only University of Rochester Faculty to be a member of the National Academy of Science, the National Academy of Engineering, and a fellow of the American Academy of Arts and Sciences. Conwell joined the University of Rochester as an adjunct professor in 1990 and then became a full-time professor in the Department of Chemistry after her retirement from Xerox in 1998.

Provost Fellowship

2018: Jackson Hernandez

The goal of the Provost Fellowship is to broaden and increase the diversity of our graduate students in doctoral programs by attracting the most promising



students from backgrounds that have been historically underrepresented in a particular discipline. Nominees for the fellowships must be US citizens or permanent residents. Specific criteria for determining diversity and selecting nominees will depend on each program, but may include ethnicity, race, gender, or disabilities.

GRADUATE AWARDS

Outstanding Graduate Student Award

2018: Lauren VanGelder

The Outstanding Graduate Student Award was established at the request of an alumnus who wanted to recognize excellence in research, leadership, and service by a senior graduate student. Winners will show not only a passion for learning and a steadfast diligence in the research lab, but also a dedication to teaching and mentoring, and a commitment to helping his/her community. The award consists of a medal, a cash prize and the winner's name on a plaque to be placed in the Chemistry Department Office. Recipients are recognized at the Chemistry Awards Get-Together the fall semester.



W.D. Walters Teaching Award

2018: Emily Edwards, David Vargas, Georgios Alachouzos, Trevor Tumiel, Andrew Kauffman (not pictured)



This award recognizes outstanding undergraduate teaching by graduate teaching assistants. This award emorializes the late Professor W.D. Walters and the standards of excellence and achievement exemplified by him. It also recognizes our appreciation for the commitment and achievements of the awardees.

ACS Women Chemists Committee/Eli Lilly Travel Award

Brittney Petel



In addition to financial support, the award provides networking opportunities for recipients who attend an ACS national meeting. The WCC hosts a poster session and reception for awardees at each national meeting. In addition, awardees are invited to the WCC Luncheon where they receive recognition. The luncheon also provides a valuable networking opportunity as awardees sit at the head tables along with ACS governance and WCC members. Lastly, awardees are invited to a private dinner with WCC members which is generously sponsored by the ACS Executive Director.

ACS Travel Award

Inorganic Division: Viktoria Steck Organic Division: Antonio Tinoco Valencia





With support from this award, Viktoria and Antonio both attended the 255th ACS Meeting in New Orleans, and gave poster presentations of their research.

Elliot and Laura Richman Travel Award

Georgios Alachouzos

This fund was established by the Richmans to enable a graduate student to attend and presnr thier research at a regional or national meeting. George used the funds to support his travel to the Gordon Research Conference on Organic Reactions and Processes.



Best Graduate Student Oral Presentation in Organic Chemistry

Antonio Tinoco Valencia



Antonio Tinoco Valencia (Fasan Group) was awarded "Best Graduate Student Oral Presentation in Organic Chemistry" at the 2018 Society for Advancement of Chicanos/Hispanics and Native Americans in Science (SACNAS) National Diversity in STEM Conference. This year the three day (10/11-10/13) conference was held in San Antonio, TX where SACNAS awarded 105 graduate and undergraduate underrepresented minority students for their research and presentation skills. The Presentation Awards recognize the next generation of scientists and STEM leaders for exemplary science, while giving visibility to their investigations and home institutions.

ACS 2018 PHYS DIVISION POSTDOCTORAL RESEARCH AWARD



Dr. Bing Gu

Dr. Bing Gu has been named as one of four recipients to win a 2018 Young Investigator Award by the Physical Chemistry division (PHYS) of the American Chemical Society (ACS). Each year the PHYS division recognizes four young researchers for their work as postdoctoral fellows (two for theory and two for experiments). The winners are invited to speak about their research at the Fall ACS meeting in August in Boston.

This award was given for Dr. Bing Gu's postdoctoral work in the Franco group developing decoherence timescales,

new methods in quantum dynamics, and investigating the effective properties of matter driven far from equilibrium.

ARKAJIT MANDAL AWARDED BEST POSTER AT CECAM AND "COKERFEST"



Arkajit receiving best poster award at Cokerfest

Arkajit Mandal, a graduate student in the Huo Group, was awarded two best poster awards, one at the "Path Integral Quantum Mechanics" school hosted by Centre Européen de Calcul Atomique et Moléculaire (CECAM) and the other at the "Cokerfest" held at Boston University, for the development of the Quasi-diabatic scheme for on-the-fly quantum dynamics propagation.

In the summer of 2018, CECAM hosted a school on Path Integral Quantum Mechanics (PIQM) at Laussane, Switzerland. About 50 students from 40 institutions and 15 countries participated in the PIQM summer school and

presented posters, with one best poster prize and three runner-ups. At the "Cokerfest", a special symposium honoring Professor David F. Coker's contribution to theoretical chemistry at Boston University, thirty graduate students and postdocs in the field of theoretical and computational chemistry presented posters, and two were awarded the best poster prizes sponsored by the Journal of Physical Chemistry A/B/C.

Faculty Publications January 2018 - December 2018

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Staff Highlights

Welcome to New Staff!

Barb Smith Accounting Bookkeeper

Barb came from Xerox to join the University of Rochester in March of 2019 as an Accounting Bookkeeper for the Chemistry Department. Barb grew up locally and received a B.S. in Accounting from SUNY Geneseo. She lives in Churchville with her cat, Spike.



Tessa Baker NMR /Safety Coordinator

Tessa received her Ph.D. in inorganic chemistry from the University of Rochester in 2018. Her research in the Neidig group focused on iron catalyzed C-H functionalization which involved using many different spectroscopic techniques. In her



new position on the technical staff as the NMR director and safety officer, Tessa is able to continue working with spectroscopy and instrumentation as she manages the NMR facility. In her role as safety officer, she gets to lay the ground work for making our department a safer environment for everyone. When she isn't working, Tessa enjoys spending time with her two dogs and husband. She also enjoys traveling, playing board games, and baking.



Staff outing on the Canandaigua Lady - Summer '18:

Row 1: Todd Krauss, Evelyn Sucy-Caffery, Robin Clark, Valerie Drake Row 2: Elly York, Jalil Shojaie, Pete Serrino, Randi Shaw, Barb Snaith

Row 3: Deb Contestabile

Row 4: Doris Wheeler, Ken Simolo, Linda Boyle

Row 5: Diane Visiko, Gina Eagan, Lynda McGarry



Terry "Ted" O'Connell 35 years:

Donna Dolan 30 years:

Ken Simolo

Deb Contestabile 20 years:

Anna Kuitems 15 years:

Don Batesky Tribute



Don Batesky in one of his favorite places- the chemistry lab.

The Department of Chemistry will greatly miss the humor and unmatched chemistry skills of senior research associate **Don Batesky.** He left this world at the proud age of 86 on September 19, 2018, leaving behind a legacy of love with his family as well as invention and innovation with the scientific community.

Born to Polish and Prussian immigrants Harriet Mietus and Philip Batorzynski, Donald was a lifelong resident of Irondequoit NY, living in the same home on Hudson Avenue for over 60 years. A graduate of Purdue University in the early 1950s, Donald was a life-long lover and practitioner of organic chemistry, having recorded some 4,000 chemical inventions and 100s of patents in his career with Kodak, Aldrich, and the University of Rochester. He spent a good portion of the 1990s in 'semi-retirement' to help raise his grandson, often attending local sports events, fishing, or enjoying the outdoors, before returning to the laboratory.

Citing his motivations as "Love and chemistry," Don faced his share of hardships in life, all the while keeping smiling and laughing as cornerstones of his personality. Donald was happily married to his first wife Dorothy for 46 years. After Dorothy's passing, Don married his second wife Joan Ayers, losing her as well to cancer after only a few years. Don then united with girlfriend Sally for some time, unfortunately losing her as well to cancer. He dedicated his remaining days to researching and experimenting with various compounds in the labs to combat the diseases that took all three women from him. Don is survived by his daughters, Donna (Jerry) Mandell, Wanda (John) Usselman; grandson, Chris (Erin) Mandell; brother, Richard (Kathy) Batesky, several great-grandchildren and several nieces and nephews. He lived, loved and laughed alongside countless friends, colleagues, students, and family, and was a constant source of happiness, inspiration and humor to all that knew him.

Don started as a production chemist at Kodak, working for the company's Eastman Organic Chemicals line. When outside companies requested chemicals not found in Kodak's catalogue, Batesky would make them as custom jobs, 10 or 20 grams at a time. "I did 11,000 literature searches and made 3,000 chemicals in 15 years, which is one per working day," he says. "I held the record with 22 lab notebooks. Hundreds of the chemicals he custom produced were subsequently added to Kodak's catalogue. He climbed the management ladder to operations manager, and after a brief retirement, Batesky worked as a contract chemist for the Aldrich Company for 15 years. He spent many of those years working alongside two other former Kodak chemists in leased laboratory space in Hutchison Hall. After his contract with Aldrich expired, Don worked for four years in Dan Weix's lab and, at the age of 85, Don discovered a new solution to a long-standing problem in purification to remove triphenylphosphine byproduct by adding zinc chloride. An article (J. Org. Chem. 2017 82, 19, p.9931-9936) describing this procedure was selected as an "editor's choice," and was the seventh-most read article in the journal for the previous 12 months. Since 2017, he had been splitting his 25-hour week working with Bob Boeckman and also with the Optical Materials Laboratory at LLE to synthesize a series of glassy liquid crystal (GLC) materials.

Working with Don for the past four years has been a wonderful experience," Weix says. "With so much experience in the lab, Don could make anything we dreamed up and even dreamed up his own ideas. Equally important has been the experience and enthusiasm he brings to the job." Don enjoyed working with students who represented the up-and-coming generation of chemists. Two of the many graduate students that were very close to Don, Astrid Olivares and Tarah DiBenedetto, will miss him and his cheerful smile, as will all of us who were lucky enough to hear his stories and perhaps be the recipient of an extra donut. Astrid wrote "Donald Batesky was a wise loving man and a passionate chemist. Over the years, I learned many things from him and about him. Don courageously lived and loved every moment of his life. Many of us had the opportunity to hold a door, walk with him, hear his crazy Kodak memories, or attend a baseball game. He brought happiness and joy to my day every time I saw him. He is missed dearly!"

Departmental Funds

You may also donate online at: rochester.edu/giving/chemistry

Your generous support to the Chemistry Department helps provide essential funding for groundbreaking research, the recruitment of premier undergraduate and graduate students, educational resources, as well as the retention of renowned faculty members. Contributions from alumni and friends to department funds help us to continue to build upon the legacy created by decades of support created by talented faculty, students, and their families. Gifts, of any amount, that are meaningful to you are meaningful to us.

Please consider your tax-deductible gift by mailing this form to the address below, or visit the secure website above to donate by credit card. Those interested in making a contribution with appreciated securities or through a Donor Advised Fund, please contact our department liaison, **Kate Clyde** at **kate.clyde@rochester.edu** or call her directly at **585-273-2050**.

Thank you for your consideration!

Chemistry Alumni Research Fund (A00736)

This fund is a department favorite. It is managed by the Chair, which allows for a quick response to support the immediate needs of faculty, students and postdocs, enhancing the overall educational experience and research activities of the department. Please note that the department recommends support to this fund, in contrast with the Deans Fund for Chemistry, as it is under direct control of the department and allows chemistry to expand the scope of its research and teaching activities as needed.

Esther M. Conwell Graduate Fellowship* (A11000)

Esther Conwell, born in 1922, was a female pioneer in Chemistry and Physics. She joined the department's faculty in 1990 and developed the Conwell-Weisskopf theory, transforming modern computing. Esther was the only University of Rochester Faculty to be a member of the National Academy of Science, the National Academy of Engineering, and a fellow of the American Academy of Arts and Sciences. Created to honor and highlight her many scientific accomplishments, this fund supports merit-based fellowships for graduates pursuing a PhD in Chemistry with exceptional research promise. Contributions to this fund will be matched up to \$20,000 per calendar year.

Jack A. Kampmeier Endowed Fund for Peer-Led Workshop Education in Chemistry*(A00880)

Designed to continue Jack Kampmeier's nationally recognized and innovative approach to teaching Chemistry through a Peerled Team Learning Workshop model, this fund continues to support workshops and the innovative training of workshop leaders that actively engage (undergraduate) students in hands-on learning and instills problem solving in a supportive and interactive educational environment.

educational environment.		
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Alumni Update

This form is available on the Chemistry Department website under Alumni.

We would love to hear from you! If your address has changed or if you have an item of interest for the next Newsletter, please fill in the form below and return to:

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