



2017

Newsletter

*Chemistry*

UNIVERSITY of  
ROCHESTER



MELIORA

VENIUDY





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# Faculty and Staff

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## **CHEMISTRY LIBRARIAN**

Sue Cardinal

# From the Chair



Greetings to Chemistry Department students, faculty, staff and especially our alumni! This past year, my fifth as Chair of the Department, we have had some very interesting developments within Chemistry and the University that I would like to share here.

One of my major goals for the Department is to lay the groundwork for the expansion in faculty size to 26 (from the current 20) over the next 7 to 10 year timeframe and thus to concurrently and significantly strengthen our research portfolio. There are considerable costs associated with starting up a new faculty member in Chemistry, which have made accelerating faculty hiring challenging. More substantial renovations due to the age of Hutchison Hall coupled with the ever more technically challenging nature of chemistry research mean that each experimental junior faculty hire is on average a 2.5 million dollar investment by the University. With this in mind, I am thrilled to report that the administration has agreed to hire 5 chemists over the next three years (a 10-12 million dollar investment in Chemistry) as a way to jump-start our drive to 26 eventual faculty! This year we were allowed to search for a faculty member in synthetic organic chemistry as part of this hiring plan, and we look forward to completing that process soon and bringing on a new organic chemistry colleague in the spring of 2018.

The Chemistry faculty continue to be recognized for their excellence in scholarship and their exemplary teaching. In particular, we want to highlight the accomplishments of several faculty including Kara Bren, who was awarded a 2017 Edward Peck Curtis Award for Overall Excellence in Undergraduate Teaching at Commencement in May. Bill Jones won the 2017 Organometallic Chemistry Award from the Royal Society of Chemistry for discovering new methods for converting hydrocarbons into useful chemicals. Ellen Matson received a Furth Fund award from the University, which is an award for promoting research of new faculty at Rochester. Ellen also won a CAREER Award from the National Science Foundation to support breakthroughs in her research on polyoxovanadate clusters as well as innovations in her teaching. Ignacio Franco won the ACS OpenEye Outstanding Junior Faculty Award for 2017 from the Computational Chemistry Division of the ACS. And last, but certainly not least, Bob Boeckman was honored by the Rochester ACS Section for 50 years of membership. Congratulations to all!

No surprise to anyone reading this, we have some great students at Rochester. This past May, we graduated 22 seniors, which is a smaller class than usual, but which nonetheless was full of exemplary students. Our seniors upon graduating pursued a number of diverse paths including obtaining advanced degrees in chemistry, medicine and related STEM fields, and starting careers in teaching or the “real world”. We also continue to have several students take advantage of the Take-5 program to stay on campus for a 5th year. I want to make special mention of Norman Zhao (Weix Group), who was selected for NSF Graduate Fellowship Award. Going forward we will have close to 60 chemistry majors in the senior and junior classes this coming academic year, which is larger than our historical average.

I want let everyone know about an exciting undergraduate initiative that was started this year with respect to improving the undergraduate laboratory educational experience. A chronic problem in our upper level laboratory courses is the temporal disconnect between what is taught in laboratory lecture, and what a given student is working on in lab. Invariably, only a fraction of students at a given time are doing the experiment



being discussed in lab lecture. Dave McCamant is working on this problem for CHM 231 by replacing some laboratory lectures with peer-led workshops. The workshops corrected this problem by having the students read the chapter and do the workshop worksheet so that they were prepared to do the experiment.

Our graduate program continues to thrive and we are proud of the research accomplishments of our students, who are making ever more interesting and impactful discoveries, which I hope you will read about in this newsletter! Several student accomplishments are worth noting: From the Fasan group, I want to congratulate Antonio Tinoco Valencia, who was awarded a prestigious Ford Foundation Fellowship, and Hanan Alwaseem who was awarded the ACS Women Chemists Committee/ Eli Lilly Travel award which she used to attend the ACS National Meeting in Washington , D.C. Lauren VanGelder from the Matson Group was selected for a NSF Graduate Fellowship Award and was also the winner of the 2017 Richman Travel Award Fellowship. This year, Abby Freyer won our recently endowed Outstanding Graduate Student Award. Congrats to Antonio, Hanan, Lauren and Abby! Eight students have received their doctoral degrees in 2017 and our total number of enrolled graduate students is currently at 75, to go along with a dozen postdoctoral fellows. The Department welcomed a class of 19 new Ph.D. students in Fall 2017. The total number of students enrolled in the graduate program is a bit lower than recent historical norms, but I expect that we will grow to well over 100 students fairly soon to populate the groups of the five expected new hires.

Thanks to all our alumni for your continuing support of the Chemistry Department. As I mentioned last year, but which bears repeating, our “Chemistry Alumni Research Fund” is a great resource as it enables us to pursue a number of impactful endeavors, including this year being used to support Fellowships for graduate students to support their research, education, and travel. Unlike the “Dean’s Fund for Chemistry,” which 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 2018, with events running October 4th through the 7th. We will continue to have the annual Chemistry Department Gates Happy Hour on campus in the late afternoon on Saturday October 6th 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. This past year we had a great turnout at the Happy Hour, and I sincerely hope to meet more of you around the country as I travel, or especially during your visits to Rochester in 2018!

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

Sincerely,



Todd D. Krauss  
Professor of Chemistry and Chair  
Professor of Optics

### **GIFTS OF \$100,000+**

Dr. Louis G. Lange III (B.A. '70)

### **GIFTS OF \$50,000+**

Dr. Richard S. Eisenberg and Marcia Eisenberg

### **GIFTS OF \$25,000+**

Dr. William D. Jones, Jr. and  
Heather M. Jones '81W (MSE)

### **GIFTS OF \$10,000+**

Dr. Harry B. Gray (Ph.D. '87 (HNR))  
Dr. Grace C. Hsu (M.S. '88, Ph.D. '91)  
Dr. Thomas J. Perun (Ph.D. '63)  
James L. Robo and Meredith B. Trim  
Dr. Lewis Rothberg (B.S. '77) and  
Dr. Shelby Nelson

### **GIFTS OF \$5,000+**

Dr. Laura K. Ackerman (M.S. '12, Ph.D. '16)  
Dr. Meagan Evans (M.S. '08, Ph.D. '11) and  
Dr. Christopher Evans (M.S. '08, Ph.D. '11)  
Dr. Ramy S. Farid (B.S. '86)  
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Kathy J. Farrar (M.S. '89W)  
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Marilyn A. Gloyer  
Dr. Elliot Richman (B.S. '70, Ph.D. '75) and  
Laura K. Richman  
Dr. Meihua Shen (M.S. '86, Ph.D. '90)  
Dr. Margaret May-Som Wu (M.S. '74, Ph.D. '76)  
and Dr. Wu-Yong Wu (Ph.D. '74)

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Dr. Walter Cooper (Ph.D. '57)  
Satenik Farid (B.S. '79, M.B.A. '83) and  
Dr. Samir Farid  
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Dr. George G. Stanley (B.S. '75) and Sally Hunter  
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Dr. Helen O. Leung  
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Dr. Robert S. Knox (Ph.D. '58) and  
Myrta B. Knox (M.M. '54E)  
Dr. Thomas R. Krugh and Rosemary Krugh  
Dr. John S. Kruse ('82, '89M(Ph.D.), '90M(MD))  
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Dr. Frederick D. Lewis (Ph.D.'68)  
Dr. Margaret Logan (M.S.'72, Ph.D.'82, Flw'88)  
Dr. Thomas A. Montzka (Ph.D.'62) and  
Joanne Montzka  
Dr. Paul C. Naegely (M.S.'77, Ph.D.'79) and  
Stella Naegely  
Dr. James B. Philip, Jr. (M.S.'78, Ph.D.'81)  
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Dr. Joanne M. Bevilacqua (M.S.'90, Ph.D.'94)  
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Slatomir Christow (B.S.'93, B.A.'93) and  
Lori Christow  
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Todd W. Crane (B.S.'94) and Laura Crane  
Dr. Arthur W. Dimock (Ph.D.'73) and  
Christine Dimock  
Dr. Steven A. Dombchik (B.S.'64)  
Dr. Richard English (B.S.'65)



Marble Meliora Panel (Hawkins Carlson room) (J. Adam Fenster)

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 Charlotte Klein (M.M. '63E)  
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 Dr. Stephen L. Teitel and Ruth A. Teitel  
 Kelsey N. Tuttle (B.A. '16)  
 Dr. Maria L. Sevilla-Wee (M.S. '70) and  
 Dr. Victorio T. Wee (M.S. '69, Ph.D. '74)  
 Dr. Richard Zallen  
 Norman Zhao (B.S. '17, B.A. '17)

## CONTRIBUTIONS IN MEMORY OF.....

### PROFESSOR ESTHER CONWELL

Ms. Rochelle Abkowitz  
 Mr. Robert Alfano  
 Dr. Ray and Karen Baughman  
 Dr. Richard and Marcia Eisenberg  
 Dr. James and Kathy Farrar  
 Dr. Rudi Fasan and Dr. Francesca Vitali  
 Dr. Alison Frontier and Dr. Harry Stern  
 Dr. Mala Ratan Gupta and Mr. Surendar Jeyadev  
 Dr. William Jones and Heather M. Jones  
 Dr. Kathryn E. Knowles  
 Dr. Robert and Myrta Knox  
 Dr. Thomas and Rosemary Krugh  
 Dr. Frederick D. Lewis  
 Dr. David and Caroline McCamant  
 Dr. Joanna Olmsted and Dr. Douglas Turner  
 Dr. Shanlin Pan and Yinghui Liu  
 Dr. Mark A. Ratner  
 Dr. Stephen and Ruth Teitel  
 Dr. Dan and Bonnie Watson  
 Dr. Richard Zallen

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 Dr. Noal and Ann Cohen

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 Scott Kampmeier and Julie Eklund  
 Dr. John S. Kruse  
 Dr. Thomas J. Perun

### PROFESSOR NABI MAGOMEDOV

Dr. David J. Hart  
 Dr. Andrei Burnin and Irina Burnina





### **THOMAS J. PERUN ENDOWED SCHOLARSHIP IN CHEMISTRY**

Thomas Perun retired in 1996 after a 33 year career in pharmaceutical research and management at Abbott Laboratories in Illinois. He received a B.S. in Chemistry from Rensselaer Polytechnic Institute in 1959 and his Ph.D. in organic chemistry from the University of Rochester in 1963, where he worked with Prof. D. Stanley Tarbell on the synthesis and novel rearrangement of compounds related to podophyllotoxin. His career at Abbott began with work on the antibiotic, erythromycin, where he determined the conformation of this important antibiotic, and developed the information that led to a number of useful derivatives in the clinic. He progressed through the management of antibacterial research, cardiovascular research, and ended as Vice President of Drug Design and Delivery. In this latter position, he had responsibility for developing the structure-based drug design group involved in the early identification of drug targets and lead molecules.

Since his retirement he has been involved with professional chemistry organizations such as the American Chemical Society and the International Union of Pure and Applied Chemistry. He was Chair of the ACS Division of Medicinal Chemistry in 1997, and continued on the Executive Committee in various functions. He recently completed a four year term as President of the IUPAC Division of Chemistry and Human Health, a worldwide organization dedicated to providing information and tools for chemists to accomplish their work on solving health problems, particularly in countries that need help in their research activities.

He has been a regular contributor to the Chemistry Department at the University of Rochester with particular interest in the Jack Kampmeier Peer-Led Workshop Education in Chemistry. He was made a Charter Member of the George Eastman Circle by President Seligman, and recently established the Thomas J. Perun Endowed Scholarship in Chemistry as a way to encourage bright young students to enter careers in chemistry.

## **CONTRIBUTIONS IN HONOR OF.....**

### **PROFESSOR JOSEPH P. DINNOCENZO**

Satenik Farid (B.S. '79, M.B.A. '83) and  
Dr. Samir Farid

### **RICHARD S. EISENBERG ENDOWED FUND**

Dr. Barbara J. Burger (B.S. '83)  
Dr. Richard S. Eisenberg and Marcia Eisenberg  
Dr. Ramy S. Farid (B.S. '86)  
Dr. James M. Farrar and  
Kathy J. Farrar (M.S. '89W)  
Dr. Harry B. Gray (Ph.D. '87 (HNR))  
Dr. William D. Jones, Jr. and  
Heather M. Jones '81W (MSE)  
Dr. Clifford P. Kubiak (M.S. '77, Ph.D. '80) and  
Pamela P. Kubiak  
Dr. Mark D. Marshall (B.S. '79) and  
Dr. Helen O. Leung  
Dr. Gordon J. Miller, Jr. (B.S. '82) and  
Irmgard M. Schewe-Miller  
Dr. Susan M. Oldham (Ph.D. '99)

### **ANDREW S. KENDE PROFESSORSHIP IN CHEMISTRY**

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Dr. Barbara E. Staub (B.A. '76, B.S. '76) and  
Donald Mitchel  
Dr. Karel M. Brands (Flw '92 )  
Dr. Paul C. Naegely (M.S. '77, Ph.D. '79) and  
Stella Naegely  
Dr. Margaret Logan (M.S. '72, Ph.D. '82, Flw '88)

### **LOUIS AND DOROTHY LANGE PROFESSORSHIP IN CHEMISTRY**

Dr. Louis G. Lange III (B.A. '70)

### **DR. THOMAS J. PERUN ENDOWED SCHOLARSHIP IN CHEMISTRY**

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

## MARGARET AND WUU-YONG WU CHEMISTRY RE-SEARCH ENDOWMENT

Dr. Margaret May-Som Wu (M.S. '74, Ph.D. '76)  
and Dr. Wu-Yong Wu (Ph.D. '74)

## MATCHING/ CORPORATE GIFTS.....

American Endowment Foundation  
Chevron Corporation  
ExxonMobil Foundation  
GSK  
Goldman Sachs & Company  
IBM Corporation Matching Grants Program  
Lam Research Foundation  
Pfizer Foundation Matching Gifts Program  
Texas Instrument, Inc.  
Xerox Foundation/Xerox Co.

## FOUNDATIONAL

MBL Family Foundation

## NOT-FOR-PROFITS

Fidelity Charitable Gift Fund  
Network for Good

## GIFTS FROM CORPORATIONS

Novartis  
Wyndham Worldwide  
Abbott Laboratories

## DR. FREDERICK LEWIS FUNDS NEW COLLEGE UNDERGRADUATE TEACHING AND RESEARCH MENTORSHIP AWARD



*Dr. Frederick Lewis*

**Frederick Lewis (Ph.D. Chemistry, '68)** was surrounded by mentors while working toward his doctorate in organic chemistry at the University. "My Ph.D. advisor was William Saunders," Lewis says. "He was wonderful, a hands-off mentor who let me go at my own speed. Two other professors, Jack Kampmeier and Marshall Gates, were role models for what an academic scientist should be. All three made an impact on me."

Although Lewis left Rochester 50 years ago to embark on what would become a 48-year career as a chemistry professor at Northwestern University, he has remained in touch with Rochester's chemistry department and remembers the inspiration he felt on campus. "I wanted to give something back," he says.

In 2017, Lewis and his wife, Susan Rice Lewis, funded a new award, the College Award for Undergraduate Teaching and Research Mentorship, to recognize a tenured faculty member in Arts, Sciences & Engineering who excels as a scholar, teacher, and mentor of undergraduate students. It salutes those tenured faculty members who teach large, introductory classes, as well as advanced seminars, independent study projects, and mentor research experiences, especially those that involve laboratory training in the sciences and engineering. "Teaching awards are almost always about classroom teaching," Lewis says. "To me, it's so important that we mentor students who will be future scientists, and that's done more in the lab than the classroom. The classroom is where you get students interested in going to a lab. The lab is where you get them engaged."

To our delight, the faculty member who was chosen as the recipient of this inaugural award was none other than Associate Chemistry **Professor David McCamant**. Over the course of the last 12 years, Dave has taught a large service class (General Chemistry - CHM132) for three semesters, the large General Chemistry Laboratory lecture (CHM131L) once and our advanced laboratory for chemistry majors, Chemical Instrumentation (CHM231 and CHM231W) eleven times. Through those courses, he has taught 1,324 students in the CHM131/132 introductory series and 271 advanced chemistry majors. Dave has worked with 21 different students, producing 12 different senior theses and 4 peer-reviewed publications with undergraduate authors.



# In Memoriam

*The Department of Chemistry  
mourns the passing of:*

John L. Barg (B.S. `46)

Dr. Gary W. Byers (Ph.D. `69)

Dr. Lloyd H. Conover (Ph.D. `50)

Dr. Harry N. Cripps (B.S. `48)

Dr. Carl Wesley Garland (B.S. `50)

Dr. Robert Gomer (Ph.D. `49)

Dr. David R. Herrick (B.S. `69)

Dr. Andrew Kende (faculty)

Dr. John William Lawrow (B.A. `48)

Dr. Charles H. Marino  
(B.S. `50, RES `57)

Dr. Dan Neuberger (Ph.D. `54)

Gordon M. Rose (B.S. `59)

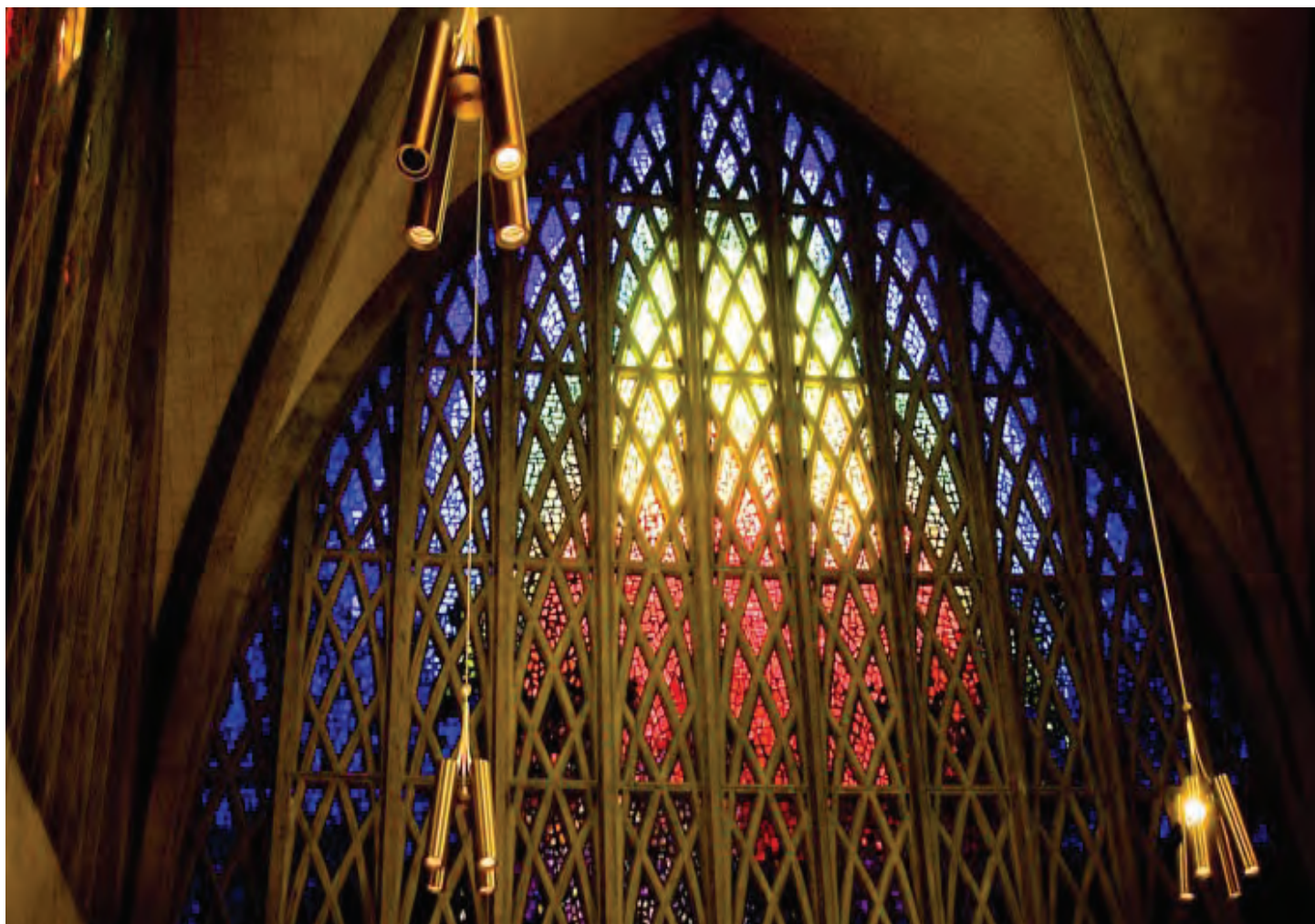
Dr. Faith Suzanne Rothermel  
(B.A. `89)

Ival Otis Salyer (B.A. `41)

Dr. Anthony F. Saturno (B.S. `54)

Dr. Peter Michael Stacy (Ph.D. `68)

Dr. David J. Wilson  
(faculty 1957 to 1969)



## In memory of Chemistry Professor Emeritus Andrew S. Kende

February 20, 2018



It is with great sadness that we share the news that Professor Andy Kende passed away suddenly on the 20th of February, 2018. He was 85 years old. Andy Kende was the Charles F. Houghton Professor of Chemistry, Emeritus and a former Department Chair. At Rochester, Andy had the

reputation for demanding scientific excellence and would not settle for less than the pursuit of science at the highest level. He mentored over 50 postdocs and 50 students during his career.

Andrew Kende entered the College of the University of Chicago at 16. His research career started under R.B. Woodward at Harvard University, where his doctoral thesis research elucidated new pathways for the reactions of aliphatic diazo compounds with ketenes and led to the first spectroscopic characterization of pure cyclopropanone. During an NRC-American Cancer Society Postdoctoral Fellowship (1956-57) with D.H.R. Barton of Glasgow, he demonstrated the structure of the major photoisomerization product of dehydroergosteryl acetate, an excursion into natural products which continued during his early years at Lederle Laboratories.

In 1968, Kende accepted an appointment as Professor of Chemistry at the University of Rochester. At Rochester his research program focused on two principal themes: pericyclic reactions and total synthesis. During his time at Rochester Kende's work on pericyclic reactions included the photochemistry of  $\beta,\gamma$ -enones and homoconjugated dienones, singlet oxygen chemistry, carbene reactions, rearrangements of cyclic polyenes, methylenecyclopropane isomerization and fragmentation, and the chemistry of isobenzofurans, mesoionic oxyallyl species, and phenalene derivatives. His studies in total synthesis include the construction of the antineoplastic alkaloid camptothecin from furfural, new methods for nucleophilic acylation and transition metal coupling reactions, development of selective photochemical methods in synthesis and new routes to

the anthracycline antibiotics, the alkaloids dendrobine and sesbanine, and to the intricate tricyclic framework of the taxane diterpenes.

As Bob Boeckman recalls, "In 1980 Andy Kende recruited me to Rochester to join he and Dick Schlessinger as part of a group doing complex molecule synthesis. I will always be grateful to him for this opportunity which has done so much for my career and me personally. Andy demanded excellence from all of those around him; students, staff, and faculty. His vision, imagination, and vast knowledge of organic chemistry were a valuable resource and set a standard which I tried to emulate. His selfless service to the field of organic chemistry was exemplary, a standard for all to strive for."

Professor Kende's research led to a 1978 Guggenheim Fellowship and to numerous invited lectures, including several Gordon Conference lectures, NSF Workshops in Natural Products Chemistry (1972 and 1974), and the International Symposium on Anthracycline Chemistry (Winnipeg, 1978), as well as plenary lectures at the Royal Society of Chemistry (Cambridge, England, July, 1983), the International Conference on Heterocyclic Chemistry (Tokyo, August, 1983), and the Medicinal Chemistry Symposium (Cambridge, England, September, 1983). In 1986, he was awarded a Japan Society for Promotion of Science Fellowship. Professor Kende also received a Cope Senior Scholar Award in 2003.



During his 50-plus years as a member of the American Chemical Society, Andrew Kende has made significant contributions to the science of organic chemistry in its broadest sense. Andrew Kende will be missed by not only us here at Rochester, but also the greater chemistry community worldwide.



## Lloyd H. Conover (Ph.D. '50)

March 11, 2017



Lloyd H. Conover, a chemist whose breakthrough invention of one of the most effective and widely prescribed antibiotics, tetracycline, led to a whole new approach to developing such drugs, died on March 11, 2017 in St. Petersburg, Fla. He was 93.

Lloyd Hillyard Conover was born on June 13, 1923, in Orange, N.J. His father, John, was a lawyer; his mother, the former Marguerite Anna Cameron, was an artist. His interest in chemistry began in childhood when he watched his father mix cement to repair a retaining wall.

Lloyd entered Amherst as a freshman in 1941. Along with many of his classmates, he took time off from his studies to serve in the military during World War II, marrying Virginia Rogers Kirk in New Orleans just before shipping out to the Pacific. Lloyd served as executive officer on an LST (landing ship tank) during the war, returning to Amherst and graduating in 1947.

Lloyd earned his doctorate in Chemistry from the University of Rochester in 1950 with research advisor Dr. D. Stanley Tarbell. Dr. Conover started his research at Pfizer in Brooklyn in 1950, when pharmaceutical companies, spurred by the success of penicillin against battlefield infections during World War II, were racing to find new antibiotics. Most early antibiotics were naturally occurring chemicals produced by microorganisms that lived in soil or on decaying fruit; the strain of penicillin used to protect wounded soldiers came from a moldy melon.

In 1952, Lloyd invented the broad-spectrum antibiotic tetracycline. Testing revealed that the drug was more strongly therapeutic with fewer side effects than both Terramycin and Aureomycin. Tetracycline became for a time the world's leading antibiotic, saving many lives. The first drug made by chemically altering an existing antibiotic—which until then were created by growing molds—Lloyd's discovery opened the door to the vast potential in man-made antibiotics. A 1992 inductee of the National Inventors Hall of Fame, he has approximately 300 patents in his name.

Dr. Conover spent his entire career at Pfizer. He went on to help invent Pyrantel and Morantel, which are used to treat parasitic worm infections, and rose through the company's executive ranks to become research director at Pfizer Central Research in Sandwich, England, in 1971. He retired as a senior vice president in 1984.

(Text is from the NY Times and The Washington Post obituaries)

## Carl W. Garland (B.S. '50)

July 11, 2017



Carl W. Garland, professor emeritus in the MIT Department of Chemistry, died Tuesday, July 11, 2017 at the age of 87. Born on October 1, 1929 in Bangor, Maine, Garland was a resident of Lexington, Massachusetts.

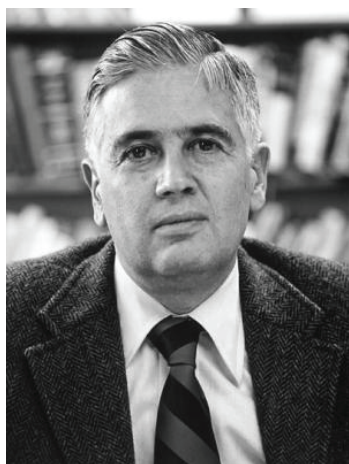
He completed his undergraduate studies at the University of Rochester in 1950, and went on to receive his Ph.D. from the University of California at Berkeley in 1953. He joined the faculty at MIT later that year as an instructor in the Department of Chemistry. Garland was a professor of physical chemistry in the department for over 40 years, until his retirement in 1997. His early teaching activity with former Professor David Shoemaker resulted in the laboratory textbook "Experiments in Physical Chemistry." Currently in its 8th edition with new co-authors, the text has been widely used across the country.

Garland held visiting professor appointments across the globe, including the universities of Bordeaux, Paris, Rome, and Cambridge; Israel's Ben Gurion University of the Negev; and Belgium's Katholieke Universiteit Leuven. In addition, he served as a scientific editor of the journals Optics and Spectroscopy and Liquid Crystals. He was an A.P. Sloan Fellow (1954-1960), a Guggenheim Fellow (1963-1964), and a fellow of the American Academy of Arts and Sciences.



## Robert Gomer (Ph.D. '49)

December 12, 2016



Prof. Emeritus Robert Gomer, a chemical physicist who pioneered techniques for studying molecules and taught at the University of Chicago for nearly a half-century, died Dec. 12, 2016 at the age of 92. Gomer was born on 24 March 1924 in Vienna. He left for the UK in 1938 as part of the child transport rescue effort,

and in 1940 he went to the US to meet his parents, who were already there. He earned his B.A. from Pomona College in 1944 and his Ph.D. in chemistry from the University of Rochester in 1949 under the direction of W. Albert Noyes. He then worked for a year on molecular chemical kinetics as a postdoctoral fellow with George Kistiakowsky at Harvard University.

From there Gomer went to the James Franck Institute and the Department of Chemistry at the University of Chicago. He spent the rest of his career there, first as an instructor and then as a professor. From 1977 to 1983, he was director of the institute. In 1984 he was named the Carl W. Eisendrath Distinguished Service Professor; he became a professor emeritus in 1996.

He wrote *Field Emission and Field Ionization* (1961) and edited several scientific journals, including *Applied Physics*. Gomer won numerous awards for his work, including the American Physical Society's 1981 Davisson–Germer Prize in Atomic or Surface Physics, the 1989 Medard W. Welch Award from AVS, and the American Chemical Society's 1996 Arthur W. Adamson Award for Distinguished Service in the Advancement of Surface Chemistry. His other awards included the Bourke Lecturer from the Faraday Society, the Kendall Award in Colloid or Surface Science from the American Chemical Society, and the Senior U.S. Scientist Award from the A. von Humboldt Society. Gomer was elected a member of the National Academy of Sciences in 1981. He was an Atomic Energy Commission Postdoctoral Fellow at Harvard University and an Alfred P. Sloan Research Fellow at University of Chicago. He also was a Guggenheim fellow at the University of Paris, and a Fulbright fellow at the Technical University of Vienna.

Besides his scientific pursuits, Gomer had an unusually broad range of interests—in theater, culture, government policies, and other arenas—that made people seek him out at Chicago and at conferences. He was an outspoken opponent of the proliferation of nuclear weapons, and he chaired the board of the *Bulletin of the Atomic Scientists*.

## David Herrick (B.S. '69)

November 14, 2017



David Herrick died on November 15, 2017 from a sudden and unexpected heart attack three days earlier, with his wife, Ann, at his side. He was born in Lafayette, Indiana, on May 9, 1947 to Robert and Colleen (Kane) Herrick. When David was eleven, his family moved to Clinton, Connecticut.

At The Morgan School he was an excellent student who served as president of his class, made the National Honor Society, and won the Bausch & Lomb Science award. David also loved sports. He lettered in baseball, basketball, and soccer, and in his senior year the school soccer team won the State Soccer Championship. It was at Morgan that he met Ann Crowder, the love of his life.

After graduating from The Morgan School, David attended the University of Rochester, where he received a B.S. in chemistry in 1969, his specific area of interest being physical theoretical chemistry. He and Ann married just before the start of his senior year, on September 7, 1968. After graduation they moved to New Haven, Connecticut, where David attended graduate school at Yale. Their daughter, Jennifer, was born there in 1969.

David received his Ph.D. in chemistry in June of 1973, and accepted a postdoctoral position at Bell Labs in Berkeley Heights, New Jersey. In August of 1975, he, Ann, and Jennifer moved to Eugene, where David had accepted a position in the chemistry department at the University of Oregon. His research focused on theoretical chemistry and chemical physics, with emphasis on novel approaches to issues involving atomic and molecular structure. His honor and awards included: Camille and Henry Dreyfus Teacher-Scholar, John S. Guggenheim Fellow, and American Physical

Society Fellow. He enjoyed teaching, and tried to make a tough class fun. Students appreciated the help sessions he offered and the practice quizzes he posted on his web site.

He enjoyed playing the piano at various university events, including the annual chemistry department holiday dinners, and at many dean's receptions over the years. It was at Oregon that David and his family also discovered the joys of Duck football, and they quickly became season ticket holders, attending all the home games and several bowl games.

## Dan Neuberger (Ph.D. '54)

January 23, 2017



In 2016 Dan Neuberger was awarded a Lifetime Achievement Award by the Niagara Frontier Regional Camera Clubs at their annual banquet, and composed his autobiography, portions of which are included below. A video produced by his Image City Photography Gallery partner Carl Crumley for that event summarizes the full life and art of Dan

Neuberger which can be viewed on their web site.

Born 1929 in the former Yugoslavia, Dan, his parents Ann and Paul Neuberger and brother Egon, immigrated to America in 1940.

“At 16, photography discovered me, when my brother gave me his 1933 Rolleiflex. I developed a real taste for photography and have been savoring it ever since.

While at Columbia College, I was very active in the camera club. I became Chairman of Experimental Workshops, and later, President. During my college years, I was a photography counselor in private camps for two summers. I graduated Magna Cum Laude in chemistry, and a Phi Beta Kappa key. The next few harrowing years were spent at the University of Rochester getting a Ph.D. in Physical Chemistry in 1953, and then in the army, so my photographic career was put on hold.

I was then hired by Kodak and worked there as a

photographic scientist for thirty-one happy years, with fascinating research and free film. I formed a symbiotic relationship between my two great loves, the scientific and aesthetic aspects of photography, both of which required creativity. I was the first scientist to be sent for a year to the research laboratories in Paris to collaborate with our French colleagues. While at Kodak, I became very active in the Kodak Camera Club, and won gold medals in the Kodak and the Rochester International Salons of Photography. My work is in the permanent collections at the Herbert F. Johnson Museum at Cornell, the Picker Art Gallery at Colgate, Kodak Camera Club, SUNY Stony Brook, and private collections here and abroad.

For the past thirty years, my cause célèbre has been to try to make photography accepted as one of the fine arts. In 2005, I was one of the founding Partners of Image City Photography Gallery, probably the only strictly photography gallery in western New York State. We have been very successful in our goal of attracting exhibitors who had very little opportunity for exhibition in Rochester, which is touted as the “Imaging Center of the World”. In 2003, 2005, and 2007, I ran a highly



dan neuberger



successful Salon des Refuses, which accepted work rejected by the most prestigious Finger Lakes Exhibition, held in the Memorial Art Gallery.”

Dan passed away on January 23, 2017 at age 87. Image City Photography Gallery hosted an exhibit of his work in May 2017. His wit and infectious smile will be missed by everyone whose life he touched.

### **Faith Suzanne Rothermel (B.A. '85)**

*November 4, 2017*



Faith Suzanne Rothermel, PharmD., BCPS, of Belton, TX died peacefully at home surrounded by her four older sisters and family on November 4, 2017 following a brief illness. She was born on April 12, 1963 in Elmira, NY to Joseph Jackson Rothermel and Daphne Land Rothermel. She graduated from Corning-

Painted Post West High School in 1981. She received a B.A. in chemistry from the University of Rochester in 1985. She then became a professional braider working the horse show circuit throughout the eastern United States. In 2000 to prepare for pharmacy school, she resumed studies at Corning Community College, graduating as valedictorian of her class in 2001. In May 2004 she earned a Doctor of Pharmacy from the Albany College of Pharmacy, graduating summa cum laude. She then completed a Specialty Residency at Scott and White Memorial Hospital (SWMH) in Temple, TX (2004-2005) and subsequently practiced hospital pharmacy in the Investigational Drugs, Operating Room, and Intravenous Drugs Preparation decentralized pharmacies at SWMH until the present. She was named “Pharmacist of the Year” for 2017 for Baylor Scott & White Healthcare.

Faith was known for her kindness, generosity and ready smile. She was passionate about her pharmacy practice, her garden and her canine companions, Jimbo, Islay and Barley and liked nothing better than to watch her dogs compete. She was active in the Heart of Texas Retriever Club, serving as treasurer for many years.

### **Ival Otis Salyer (B.A. '41)**

*October 15, 2017*



A prominent University of Dayton researcher and retired Army Air Force sergeant has died.

Ival Salyer, 100, died Oct. 15, 2017 according to his obituary. A memorial service was held on Oct. 28 at Bethlehem United Methodist Church in Buford, Georgia.

After getting a degree in chemistry from the University of Rochester in

1941, Salyer joined the Air Force during World War II. After serving four years, Salyer returned home to marry his wife, Jane. The couple spent most of their 61 years together in Dayton, Ohio, where Salyer worked at the Monsanto Research Corp., then at the University of Dayton Research Institute. While at UDRI, he worked as a senior research scientist and helped to create a fire extinguishing foam in 1990.

Salyer’s scientific contributions are vast. His name is on more than 130 patents — including his very last one for a hybrid aircraft design after turning 98 in 2015.

His scientific work contributed to the development of the artificial heart and kidney made out of a polymer material that the body does not reject. His daughter, April Bell, said her father had a hand in developing Astro-Turf and artificial sugar, worked on stealth bomber coding, corroborated with atomic research laboratories, working on flame-retardant material and was among the scientists called in by NASA to review and make recommendations following the Challenger disaster. For all of his scientific accomplishments, her father was “a very simple person” who engaged in everyday life, Bell said. She said he found the time to volunteer with the Boy Scouts, was president of the Lions Club, made it to PTA meetings and was a leader and officer in church.



## David J. Wilson (faculty 1957 to 1969)

January 12, 2017



Former faculty member David J. Wilson passed away January 12, 2017. Professor Wilson was appointed in 1957 to the UR Department of Chemistry faculty, and rose rapidly through the ranks before moving to Vanderbilt University in 1969.

Professor Wilson's research focused on the kinetics of small molecule reactions. Wilson's early research emphasized quantum and classical theoretical methods for investigating chemical kinetics problems at the level of atoms and molecules, and included a paper that has been recognized as a landmark contribution to chaos theory.

In the 1960s, while living in Rochester, Wilson became involved in environmental advocacy when he joined efforts to remove lead paint from old houses. He also participated in a campaign to stop sewage contamination of Lake Ontario beaches from an outdated treatment plant and received a sportsman-conservationist award in 1967 for his efforts.

By the time he retired in 1995, he had published three books and about 300 journal articles, and had supervised the research projects of 34 Ph.D. students and a comparable number of master's and undergraduate researchers.



*Paper cranes tucked into the walls of the Interfaith Chapel  
(J. Adam Fenster)*



# A REMEMBRANCE OF PROFESSOR WINSTON DANAE (W.D.) WALTERS

by his daughter **Laura Walters Blanda**

*March 30, 2017*



Of course to us he was our father, Daddy, but to others he was the professor. Some called him “The Chief!” a moniker bestowed by Carl Whiteman, I think!

In addition to his intellect and high moral standards, he was a man with a deep sense of compassion for all living creatures. Growing up, we had a dog, George, who had a bad habit of chasing cars. During one incident, as George licked his wounds, my father fed him bits of roast beef that miraculously did the trick!

I remember another time when this same dog chewed a paper gum chain that I had meticulously constructed. My father comforted me, still dressed for work in his crisp white shirt! He always dressed in a suit, tie and white shirt, with a fedora; and his Movado watch, a wedding gift from my mother.

He was young when he died. Only 53, with cancer taking him from us much too soon. I was 16, my brother 14. We never had the chance to develop adult relationships with him and my memories are softened by the many years that have passed since his death in 1968! I wish that I could have seen him teach. He was very dedicated to his students and I know he took things very personally.

His grandparents immigrated from Sweden before the turn of the twentieth century and his father was one of six children raised in the Midwest during a time of opportunity and strong family ties. John, his father became a grocer and ran the business with two of his brothers. His mother’s family was from Indiana and Ethel Pyle was raised by a stepmother who was short on affection.

My father was an only child, the prized son and all focus was put on him to do well, to be educated, to succeed. He graduated from Paseo High School in Kansas City with honors. Attended Washington University in St. Louis and received his PhD from John’s Hopkins.

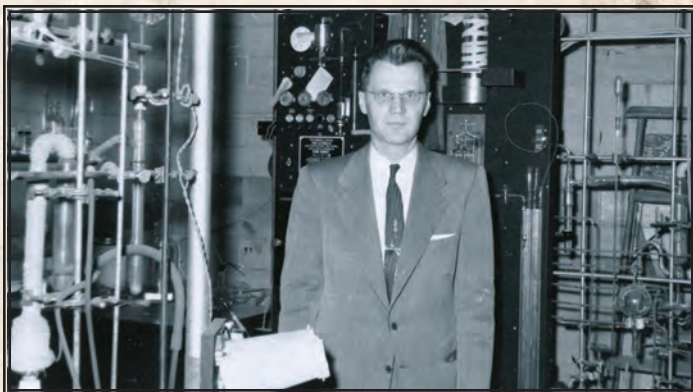
Right before World War II he was awarded a Fulbright Scholarship that enabled him to travel to Germany to study chemistry. There he learned to ski and also witnessed close up the rise to power of Hitler. During the war he worked at Dugway Proving Ground in Utah and in Washington DC where he met my mother, Elizabeth Ballard, a chemist, who also worked for the war effort.

They married in 1945 and moved to Rochester where my father was “recruited” by Dr. Albert Noyes to teach at the U of R.

After all these years I can still see his office, his desk and remember writing on the chalkboard. I can still hear the sound my brother and I made running down the hall to the stairs that led to the chem lab, the peculiar acrid smell from some experiment greeting us as we raced to see Carl...who always asked: “What did you learn in school today?”

It was a smaller world then, less intrusions, less conflict... we learned to swim on summer evenings at the university pool. We rode the lions in front of Lattimore Hall while waiting for my father to be done. We spoke with respect to his colleagues when we were allowed the privilege of visits to his office.

Now, almost 50 years later, his legacy lives on in the spirit of leadership, high academic standards and vital research. The W.D. Walters Teaching Award recognizes outstanding undergraduate teaching by graduate teaching assistants. He was a humble man but I know that every year when this award is bestowed in his name, he is proud that dedication, hard work and scholarship have been rewarded!





# Meliora Weekend 2017

The annual 2017 Marshall Gates Happy Hour was held in the afternoon on Saturday, October 14th 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 6th, 2018. Please join us this fall!



*L to R: Scott Hicks, Tad Hicks (baby), Dave McCamant, Barb Snaith, Amanda Amori, Ellen Matson Hicks, Leah Frenette*



*L to R: Jennifer Le, Maria Zambrano, David Vargas, Diego Arevalo, Hanan Alwaseem*



*L to R: Dave McCamant, Lewis Rothberg, Marcia and Richard Eisenberg, Shelby Nelson*



*L to R: Oliver Swart, Daniel Curran, George Alachouzou, Jose Alvarez - Hernandez*



*L to R: Gita Devi, Kate Clyde, Don Batesky*



*Catherine and Steven Perez*



*Lauren Bolz, Yashika Sharma, Antonio Tinoco*



# Faculty Awards

## AWARDS

### William D. Jones receives Humboldt Research Award and Organometallic Chemistry Award from the Royal Society of Chemistry



Professor William D. Jones has received the prestigious Humboldt Research Award. The award will enable him to spend up to one year cooperating on a long-term research project with specialist colleagues at a research institution in Germany.

Jones, the Charles F. Houghton Professor of Chemistry, will work with Christian Müller, a professor of chemistry at the Free University of Berlin, for six months beginning in January. Jones is interested in using rigid molecular frameworks to hold a metal atom in a precise conformation to enable specific types of dehydrogenation catalysis. Müller's work in this area will allow the exploration of new classes of pincer chemistry for this purpose.

The Alexander von Humboldt Foundation grants up to 100 Humboldt Research Awards annually to academics "whose fundamental discoveries, new theories, or insights have had a significant impact on their own discipline and who are expected to continue producing cutting-edge achievements in the future."

Jones was also the recipient of the 2017 Organometallic Chemistry Award from the Royal Society of Chemistry for finding new methods for converting hydrocarbons into chemicals found in useful, everyday products.

The award consists of £2000 and a medal. In addition, Jones is invited to deliver lectures at up to four United Kingdom universities between September 2017 and May 2018.

An example of Jones' research is a series of reactions that results in the selective conversion of ethanol to butanol, without producing unwanted byproducts.

"Butanol is much better than ethanol as an alternative to gasoline," Jones says. "It yields more energy, is less volatile, and doesn't cause damage to engines."

Jones was inspired to work in inorganic chemistry as an undergraduate researcher with Mark S. Wrighton at Massachusetts Institute of Technology (B.S., 1975). He obtained a Ph.D. degree in chemistry at California Institute of Technology (1979), working with Robert G. Bergman. He moved to the University of Wisconsin as a NSF postdoctoral fellow with Chuck Casey, and in 1980 accepted a position as Assistant Professor at the University of Rochester. He was promoted to Associate Professor in 1984 and Professor in 1987, and is now the Charles F. Houghton Professor of Chemistry.

Professor Jones has received several awards, including an Alfred P. Sloan Research Fellowship (1984), a Camille & Henry Dreyfus Foundation Teacher-Scholar Award (1985), a Royal Society Guest Research Fellowship (1988), a Fulbright-Hays Scholar (1988), a John Simon Guggenheim Fellow (1988), the ACS Award in Organometallic Chemistry (2003), and an ACS Cope Scholar Award (2009). He is a Fellow of the American Association for the Advancement of Science (2009), and a Fellow of the American Chemical Society (2010). He also has served as an Associate Editor for the Journal of the American Chemical Society since 2003. Professor Jones' research interests include organometallic research in strong C-X bond cleavage, catalysis, model studies, mechanisms, kinetics, thermodynamics, and synthetic applications.



*Prof. Jones receiving RSC award*

## Ignacio Franco Selected as Recipient of ACS OpenEye Outstanding Junior Faculty Award



Ignacio Franco, Assistant Professor of Chemistry and Physics, was awarded the ACS OpenEye Outstanding Junior Faculty Award for Fall 2017 for his proposal entitled “Atomistic modeling of electromechanical spectroscopies in molecular junctions.” The ACS COMP OpenEye Outstanding Junior

Faculty Award program provides \$1,000 to up to four outstanding tenure-track junior faculty members to present their work in COMP poster session at the Fall 2017, Washington DC ACS National Meeting. The Awards are designed to assist new faculty members in gaining visibility within the COMP community.

Professor Franco received a B.S. in Chemistry from the National University of Columbia in Bogota in 2001. He went on to receive a Ph.D. in Theoretical Chemical Physics at the University of Toronto in 2007 with Paul Brumer, followed by a postdoctoral fellowship with Mark Ratner at Northwestern University from 2008 to 2011. He then moved to the Theory Department at the Fritz Haber Institute of the Max Planck Society in Berlin, Germany to lead the research group of Matthias Scheffler until 2013 when he was appointed an Assistant Professor of Chemistry at the University of Rochester.

## Ellen Matson receives 2017 NSF CAREER Award and Furth Fund Award



Assistant Professor Ellen Matson is the recipient of a 2017 CAREER Award from the National Science Foundation for her proposal entitled “Synthesis, Characterization and Reactivity of Iron-Functionalized Polyoxovanadate-Alkoxide Clusters for the Activation of Small Molecules.”

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.

Using this award, Professor Ellen Matson and her research group will investigate the synthesis and reactivity of a family of iron-functionalized polyoxovanadate-alkoxide clusters. These hexanuclear, multi-metallic, Lindqvist clusters possess rich redox chemistry, making them ideal platforms for the mediation of multi-electron transformations pertinent to the activation of small molecules (e.g. CO<sub>2</sub>, N<sub>2</sub>, NO<sub>x</sub>, etc.). In addition to establishing a general synthetic route to access iron-functionalized polyoxovanadate-alkoxide clusters, Dr. Matson is working to develop an understanding of the electronic properties of these delocalized systems through stoichiometric redox reactivity. These research efforts are generating a unique class of metalloligands to support multi-electron transformations using first-row transition metal centers; with a focus on the ability of the metal-oxide framework to serve as a redox-active reservoir. Dr. Matson is actively engaged in multiple outreach initiatives targeted at facilitating dissemination of scientific content to young students. Matson was also a recipient of the 2017 Furth Fund award from the Provost’s Office. The Furth Fund, established through the generosity of Valerie and Frank Furth, was created to provide early career scientists with \$10,000 in research funds.

Matson earned her B.A. in Chemistry and B.S. in Science Education in 2009 at Boston University. She then moved to the Midwest to pursue her Ph.D. in Chemistry at Purdue University under the guidance of Suzanne C. Bart. During her time as a graduate student, Ellen helped expand the understanding of the synthesis and reactivity of low-valent uranium alkyl complexes. Her work culminated in a number of national recognitions, including the Iota Sigma Pi Anna Louise Hoffman Award for Outstanding Achievement in Graduate Research (2013) and the American Chemical Society Division of Inorganic Chemistry’s Young Investigator Award (2014).



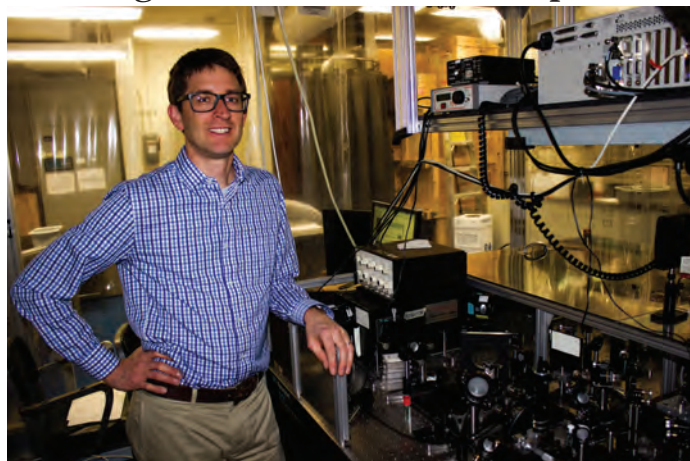
## Bren wins 2017 Curtis Award for Excellence in Undergraduate Teaching



Professor Kara L. Bren was selected as the recipient of the 2017 Edward Peck Curtis Award for Excellence in Undergraduate Teaching. The award was presented to Professor Bren at the College Commencement Ceremony on Sunday, May 21, 2017. Professor Bren received strong nomination letters from both current and former colleagues and undergraduate students. The students described her enthusiasm for teaching chemistry, and provided passionate testimonials of how she has been an enormous influence in their budding scientific careers. A common thread in all the student letters is that she deepened their interest in science, especially Chemistry, and that as a result the interactions between Professor Bren and these students were life-altering.

Professor Bren earned her B.A. in Chemistry at Carleton College in Northfield, Minnesota, where she did research with Lynn Buffington on the NMR of carbohydrates. She earned her Ph.D. in the lab of Harry B. Gray at the California Institute of Technology in Pasadena, California studying the ligand binding properties of engineered heme proteins. While earning her graduate degree, she spent time in the lab of Ivano Bertini at the University of Florence where she learned about the NMR of paramagnetic biomolecules. She continued her training as a NIH postdoctoral fellow in the lab of Gerd N. La Mar at the University of California- Davis where she performed NMR studies on paramagnetic iron-sulfur proteins. Professor Bren then started as an assistant professor of Chemistry at the University of Rochester in 1997, and became a full professor in 2008. At Rochester, the Bren group is developing biomolecular catalysts for fuel-forming reactions. Professor Bren has advised 21 Ph.D. students, 10 M.S. students, and 19 undergraduate senior thesis students.

## Chemistry Professor David McCamant wins Inaugural College Award For Undergraduate Teaching and Research Mentorship



Congratulations to Dave McCamant for being selected as the first recipient of The College Award for Undergraduate Teaching and Research Mentorship. Thanks to the generous support of Frederick D. and Susan Rice Lewis in 2017, this award recognizes a tenured faculty member in Arts, Sciences and Engineering who excels as a scholar, teacher, and mentor of undergraduate students.

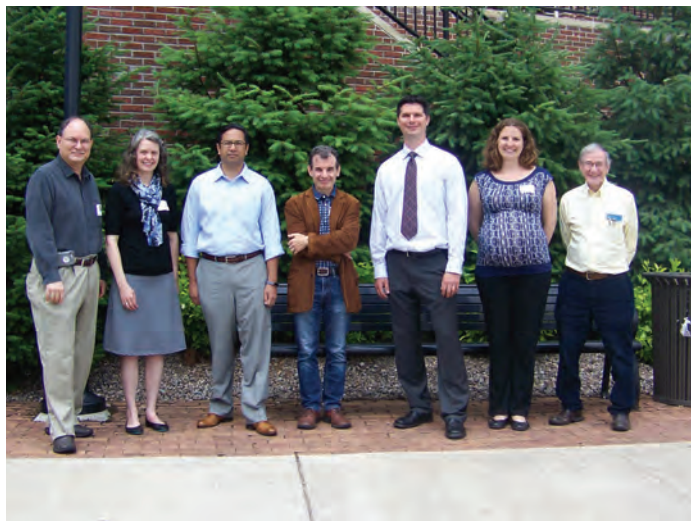
Professor McCamant received his B.A. from Wesleyan University in Connecticut and then his Ph.D. from UC Berkeley in 2004, working with Professor Richard Mathies to develop femtosecond stimulated Raman spectroscopy as a new method to collect high-resolution vibrational spectra of ultrafast photochemical events. From 2004-06, he worked with Prof. Michael Wasielewski as a postdoc at Northwestern University, studying photoinduced charge-transfer compounds. He started as an Assistant Professor at the University of Rochester in 2006 and was promoted to Associate Professor in 2012.

This award recognizes the important relationship between classroom learning and mentorship through research opportunities. It salutes those tenured faculty members who teach large, introductory classes, as well as advanced seminars, independent study projects and mentor research experiences, especially involving laboratory training in the sciences and engineering. Dr. Lewis (Ph.D., '68), whose career spanned 48 years in teaching and research at Northwestern University, said that the intent of the award is to "reward tenured faculty members who continue to fulfill the promise, every day and every year, of being outstanding teachers, mentors, and scholars."



# NIH CBI GRANT

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



*L to R: Nils Walter, Kara Bren, Omar Bakht, Joseph Wedekind, Stephen Tajc, Sarina Bellows, Doug Turner*

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.

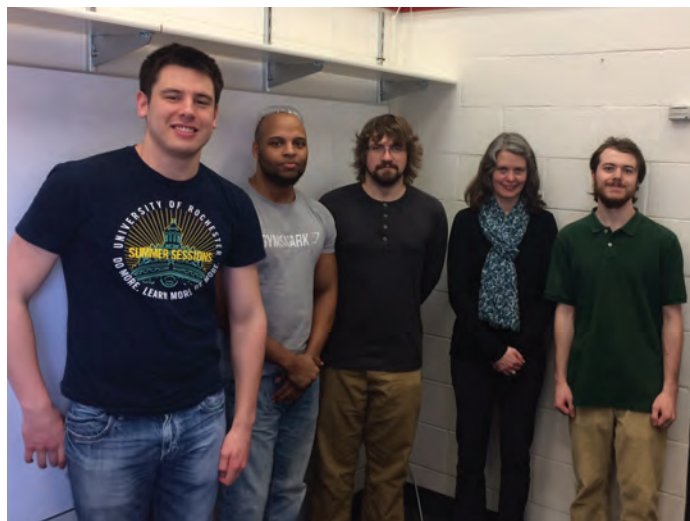
Chemistry **Professor Kara Bren** is the Program Director, and **Professors Rudi Fasan** and **Bradley Nilsson** are co-Directors. **Lynda McGarry** is the CBI program coordinator. Thirty faculty members from six departments and programs in Arts, Sciences and Engineering and in the School of Medicine 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 will include coursework on CBI science, in critical thinking, and in effective scientific communication. Trainees will 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 will receive specialized training to serve as Peer-Led Team Learning (PLTL) workshop leaders for CBI courses.

In this first year of the five year training grant, four trainees were recruited from the associated degree programs, which are Biology, Biomedical Engineering, Biochemistry, Biophysics, Chemistry, and 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.

### Congratulations to our first group of trainees!

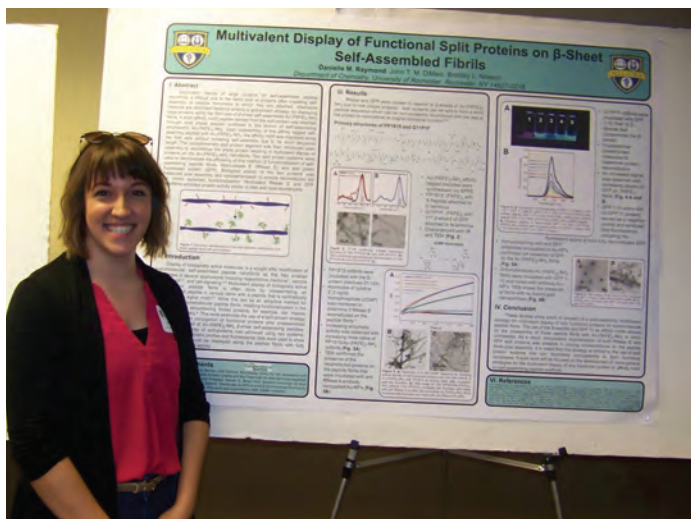
**Shukree Abdul-Rashed** is in Chemistry **Professor Alison Frontier's** research group. He is currently working on methodology for the Lewis Acid-Initiated Alkynyl Halo-Prins reaction and its applications to natural product synthesis.



*L to R: Eric Moore, Shukree Abdul-Rashed, Clyde Overby, Dr. Kara Bren, Chapin Cavender*

**Chapin Cavender** is a graduate student in the research group of **Professor David Mathews** in the Department of Biochemistry and Biophysics in the medical center. One of the projects that Chapin works on is optimizing the nonbonded parameters in the AMBER force field for classical molecular dynamics simulation of RNA molecules by fitting parameters to energies obtained from electronic structure calculations over a dataset of experimental RNA structures.

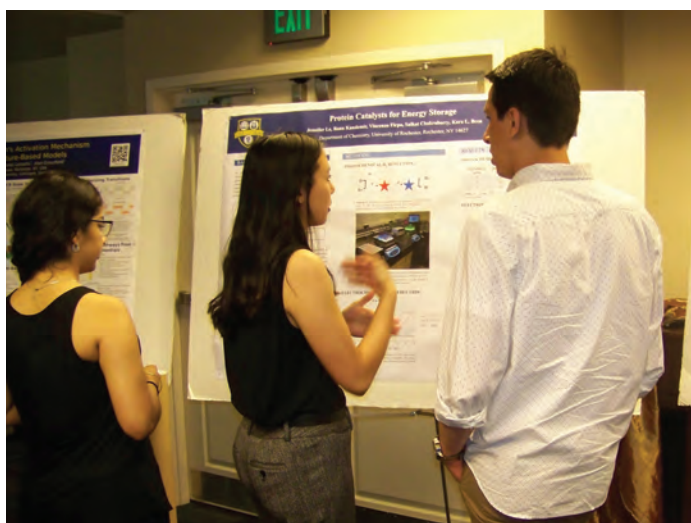
# NIH CBI GRANT



*Danielle Raymond at the poster session*



*Dinner at Staybridge Suites*



*L to R: Jasmine Gomez, Jennifer Le and Antonio Tinoco at poster session*

**Eric Moore** is a member of Chemistry **Professor Rudi Fasan's** research group. His research is focused on the design and development of myoglobin-based artificial enzymes for (asymmetric) carbene transfer reactions, a class of synthetically important transformations that are not found in nature.

**Clyde Overby** works in the research group of BME **Professor Danielle Benoit**. His research focuses on reducing the occurrence of non-specific interactions of nanoparticles with proteins in blood to enable systemic delivery of nucleotide therapeutics with nanoparticles using biomimetic, zwitterionic surface groups and investigating the replacement of pH responsive elements in the nanoparticles with peptides.

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 2017 CBI Retreat was held on June 15-16 and the keynote speaker on the first day was **Professor Nils Walter** from the University of Michigan Department of Chemistry. The title of his talk was "Single Molecules In Focus: Understanding RNA-Driven Regulation From First Principles."

The second day of the retreat, attended by 70 participants, was held at The Staybridge Suites, and included a talk by **Professor Stephen Tajc** from Nazareth College. **Dr. Tajc** also participated in the career panel discussion with **Dr. Omar Bakht** (UR Ventures), **Dr. Sarina Bellows** (SiGNa Chemistry, Inc.), and **Dr. Nils Walter** (U. Michigan).

This lively and interesting discussion was followed by lunch, a poster session, and talks by graduate students **Sreyoshi Sur** (Grossfield Group, UR Chemistry, UR Biochemistry & Biophysics), **Hong Zhu** (Dumont Group, UR Biochemistry & Biophysics), and **Eric Moore** (Fasan Group, UR Chemistry).



# Magomedov Award

## Dr. Sara Skrabalak receives the 2017 Magomedov-Shcherbinina Award

The 2017 Magomedov-Shcherbinina Memorial Prize was awarded to Sara Skrabalak on September 20th, 2017. The title of her seminar was “Function follows Form? Synthesis and Application of Metal Nanostructures.” Dr. Skrabalak is the James H. Rudy Professor of Chemistry at Indiana University – Bloomington and a recipient of both NSF CAREER and DOE Early Career Awards. She is a 2012 Research Corporation Cottrell Scholar, a 2013 Sloan Research Fellow, a 2014 Camille Dreyfus Teacher-Scholar, and recipient of the 2014 ACS Award in Pure Chemistry and 2015 Baekeland Award. In 2017 she was named both a Fulbright Fellow and Guggenheim Fellow. Her research group is developing new synthetic methods to solid materials with defined shapes and architecture then studying the structure-function relationships of prepared materials as they are applied to energy applications.



*Dr. Sara Skrabalak*

This prize memorializes the lives of Nabi, Natalya, and Amir Magomedov who lost their lives in a 2006 multi-vehicle accident. Nabi was a rising Assistant Professor of the chemistry department. His wife, Natalya Shcherbinina, was a research scientist at Bausch & Lomb. This prize is given to a young scientist who has demonstrated exceptional ability in research in early years of their first independent academic appointment with the promise of outstanding accomplishments in the future.

Dr. Skrabalak received her B.A. degree in chemistry from Washington University in St. Louis in 2002 where she conducted research with Professor William E. Buhro. She was the recipient of the Sowden Award in undergraduate research from the Department of Chemistry. She then moved to the University of Illinois at Urbana-Champaign where she completed her Ph.D. degree in chemistry in fall of 2006 under the direction of Professor Kenneth S. Suslick. There, she was the recipient of the T.S. Piper Thesis Award for her work on porous materials. She then conducted postdoctoral research at the University of Washington – Seattle with Professors Younan Xia and Xingde Li, designing nanomaterials for biomedical applications.



# PBK Visiting Scholar

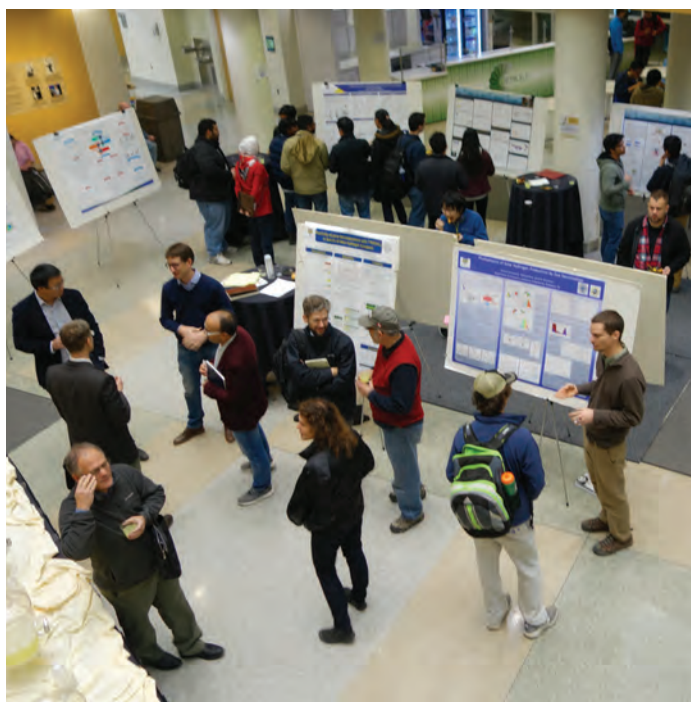
The Iota Chapter of Phi Beta Kappa and the University of Rochester Chemistry Department welcomed PBK visiting scholar Victor S. Batista, Professor of Chemistry at Yale University and Senior Editor of Journal of Physical Chemistry (JPC) to the U of R.

As part of his visit, Prof. Batista gave a public talk entitled: **“Converting Water into Fuel: Natural and Artificial Photosynthesis”**, on Thursday, Nov. 30, 2017. The room was packed, with 160 people coming from across the University and the Rochester community. Prof. Batista also spoke to Prof. Krugh’s General Chemistry course about the role that machine learning via computational neural networks can revolutionize scientific research in many disciplines and to Prof. Rothberg’s Quantum Mechanics course about a new generation of research combining classical and quantum dynamics simulations. The two-day visit inspired undergraduate researchers and spurred new ideas among faculty and graduate students.

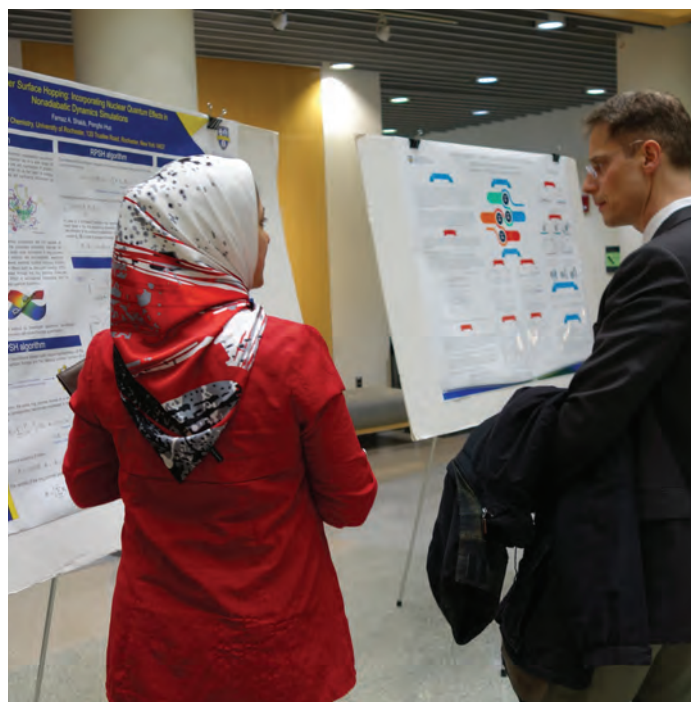


Professor Victor Batista

Victor Batista is a professor of chemistry and has served as director of undergraduate studies at Yale, 2008-2010, and as senior editor of *The Journal of Physical Chemistry* since 2011. After receiving his B.Sc. degree in chemistry at the Universidad de Buenos Aires, he continued his studies at Boston University, UC Berkeley, and the University of Toronto. His research is concerned with the development of rigorous and practical methods for simulations of quantum processes in complex systems, and with applied studies of photochemical and electrochemical processes in: proteins, semiconductor materials, aerosols, and catalysts for the chemical conversion of carbon dioxide and water. His honors include the National Science Foundation’s Presidential Early Career Award for Scientists & Engineers, the Camille Dreyfus Teacher-Scholar Award, an Alfred P. Sloan fellowship, and co-chairmanship of the 2016 Vibrational Spectroscopy Gordon Research Conference.



26 The poster session after the public lecture was well-attended and had 16 poster presenters from the Chemistry department.



Professor Batista with a student presenter at the poster session.



# PBK Visiting Scholar



*A full house at the public lecture- standing room only!*



*Professor Batista with Chemistry Professor Bill Jones.*



*Chemistry Professors Pengfei Huo, David McCamant and Ignacio Franco with Professor Batista at the poster session.*



*Prof. Matson and Prof. Hafensteiner on the tour of the bells of the Hopeman Memorial Carillon in the Rush Rhees Library tower with Professor Batista.*



*Prof. Batista presenting his lecture in Sloan Auditorium*



## Materials Science Symposium on Biomimetic & Anti-fouling Interfaces

The **Rochester Advanced Materials Science Program (RAMP)** sponsored the Frontiers in Materials Science for the 21st Century Symposium on Friday, May 26, 2017 at the University of Rochester in Goergen Hall, Sloan Auditorium. This year's topic was "*Biomimetic & Anti-fouling Interfaces*" and there were four keynote speakers, a poster session, and ten 5 minute lightning talks by invited graduate students and postdocs. The symposium organizing committee included RAMP Program Director, Chemistry Professor **Lewis Rothberg**, Professors **Andrew White** and **Alex Shestopalov** from the Chemical Engineering Department, and Gina Eagan, RAMP program administrator.

Fouling is the accumulation at interfaces of bio-macromolecules in complex media like blood or seawater. This process of accumulation gradually conceals the original surface chemistry of a material and nullifies any engineered properties. Fouling of interfaces and materials is a pervasive industrial challenge impacting fields like real-time glucose monitoring, blood clot formation on coronary angioplasty stents, degradation of maritime hulls in seawater, and membranes for desalination. This symposium brought together distinguished researchers developing novel and often biomimetic approaches to reduce and even create passive "non-fouling" materials. The goal of the symposium was to learn and foster expertise in anti-fouling in the existing work on materials at UR.

### Keynote speakers:

**Professor Kagya Amoako,**  
**University of New Haven**

"Nitric Oxide Releasing Polymer-based Systems for Anti-clotting Anti-bacterial Applications"

**Professor Milan Mrksich,** **Northwestern University**

"Combining Arrays and Mass Spectrometry for High Throughput Discovery in Chemistry and Biology"

**Professor James McGrath,**  
**University of Rochester**

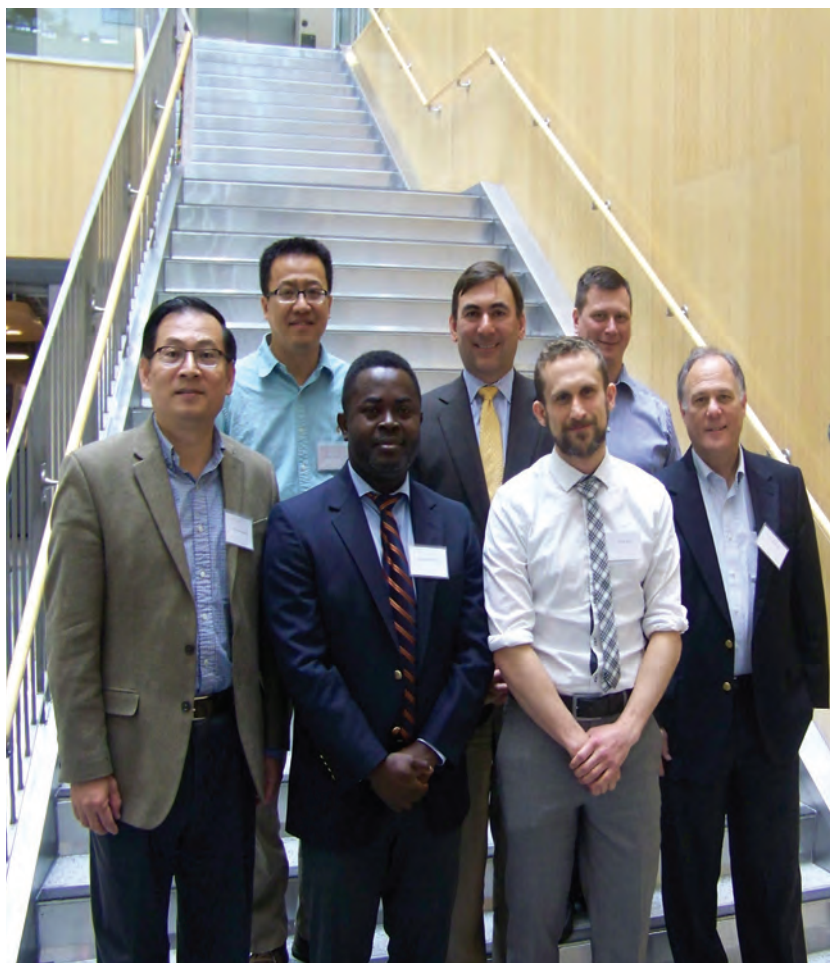
"Mechanisms of Sieving and Fouling in Ultrathin Membranes"

**Professor Shaoyi Jiang,**  
**University of Washington**

"Molecular Understanding, Design and Development of Ultra Low Fouling Zwitterionic Materials"

**Professor Jie Zheng,**  
**University of Akron**

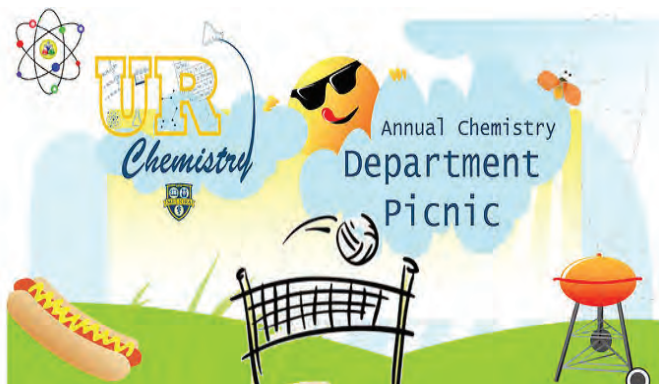
"From Fundamentals to Design of Multifunctional Soft Materials"



*L to R: Professors Shaoyi Jiang, Jie Zheng, Kagya Amoako, Milan Mrksich, Andrew White, Alex Shestopalov, Lewis Rothberg*



# Summer Picnic 2017





# Summer Picnic 2017





# REU Program 2017

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**. This summer (2017) we had 31 undergraduates participating in the REU program. The program participants included 7 international students, 10 students from other US schools and 14 UR undergraduates. 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 2017 REU Students (left to right, front to back):*

*1st Row: Hyerin Yoon, Jasmine Gomez, Ana Claudia Fingolo, Patrick Forrestel, Muhibatu Osumanu.*

*2nd Row: Shirley Zheng, Yoshimi Araki, Matthew Aquilina, Annie Stevens, Perry (Lillian) Hicks, Matthew Watrous.*

*3rd Row: Melissa Marx, Jackson Hernandez, Emma Kruger, Robbin Jang, Justin Galardi.*

*4th Row: Jiwon Han, Zachary Marshall-Carter, Gilbert Smolyak, Paul Sinclair, Jakub Vaith.*

*5th Row: Joshua Lomeo, Dominick Sarappa, Alessandro Rognoni.*

*6th Row: Noah Sims, Thomas Lyon, Pawel Wojcik, Fredrik Valgeborg.*

# International Student Research Program

In 2015, the Department of Chemistry inaugurated 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 2017 version, the Department invited six students coming from very different parts of world (UK, Poland, Italy, Sweden, South Korea, and Brazil) 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 from June 29, 2017 of the Participants in the Summer Research Experience for Undergrads Program for International Students that Ignacio coordinates:



*2017 International Summer Students with mentors and faculty advisors*

*Bottom Row (L to R): Fredrik Valgeborg (Sweden, Physical Chemistry), Sutirtha Chowdhury (Mentor), Alessandro Rognoni (Italy, Theoretical Chemistry), Katie Knowles (Advisor), Ana Claudia Fingolo (Brazil, Physical Chemistry), Mehrin Tariq (Mentor).*

*Center row (L to R): Ignacio Franco (Advisor/Coordinator), Xinyang Li (Mentor), Antonio Garzon (Mentor), Zachary Piontkowski (Mentor), Pawel Wójcik (Poland, Physical & Theoretical Chemistry), Jiwon Han (South Korea, Inorganic Chemistry), Jennifer Le (Mentor).*

*Top row (L to R): David McCamant (Advisor), Frank Huo (Advisor), Georgios Alachouzos (Mentor), Jakub Vaith (UK/Czech Republic, Organic Chemistry), Alison Frontier (Advisor).*



# Summer 2017 Outings



Last July 2017, a group of International REU visiting students, their mentors, a few advisors and co-workers went kayaking on beautiful Canadice Lake (L to R): Xinyang Li (Frank Huo's group); Barb Snaith; Zhi Wu (Visiting student in Dave McCamant's group); Sharma Yamijala (postdoc in Frank Huo's group); Katie Knowles (Assistant Professor); J.C. Olson (Assistant Professor); Ana Fingolo (International REU student from Brazil); Alessandro Rognoni (International REU student from Italy) Pawel Wocjik (International REU student from U.K.); Perry Hicks (Georgia Tech); Jakub Vaith (International REU student from Poland); Jasmine Gomez (Oswego); Jiwon Han (International REU student from South Korea); and Fredrik Valgeborg (International REU student from Sweden)



Students visiting High Falls in Rochester

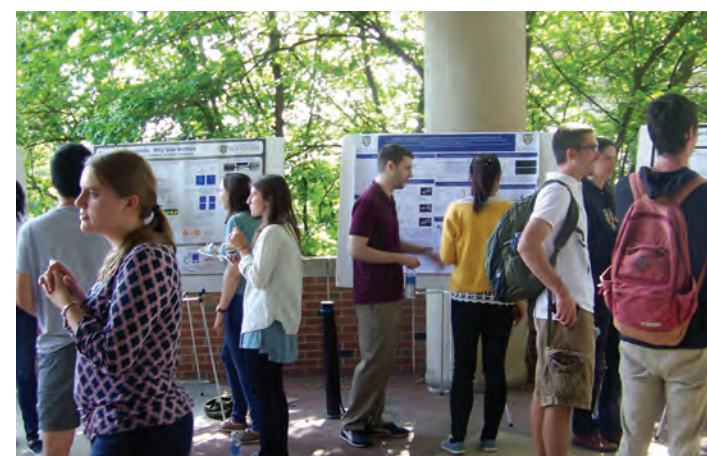
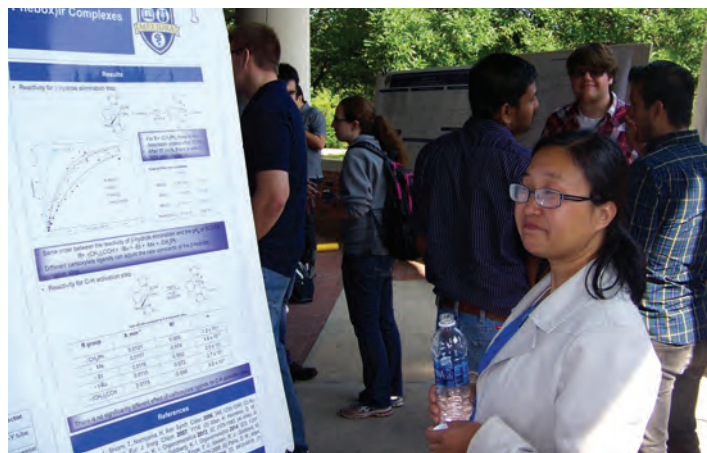
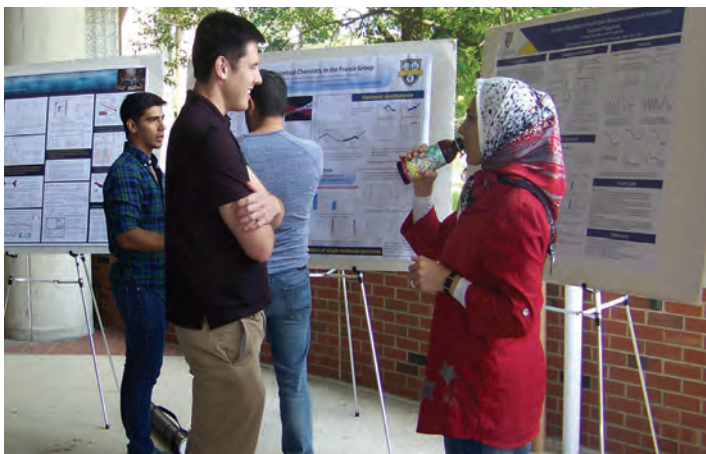
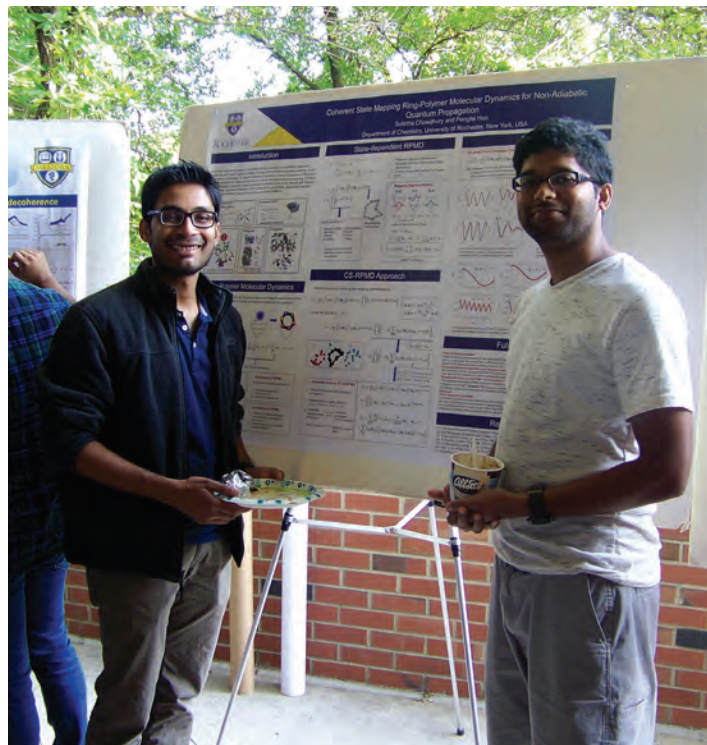
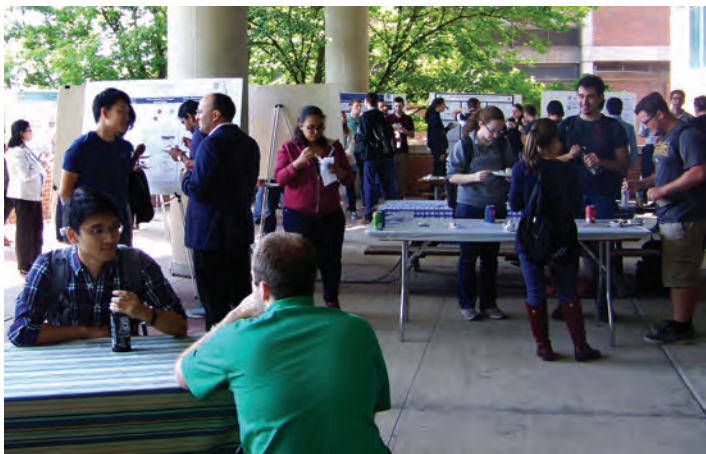


Students visiting Susan B. Anthony's grave in Mt. Hope Cemetery



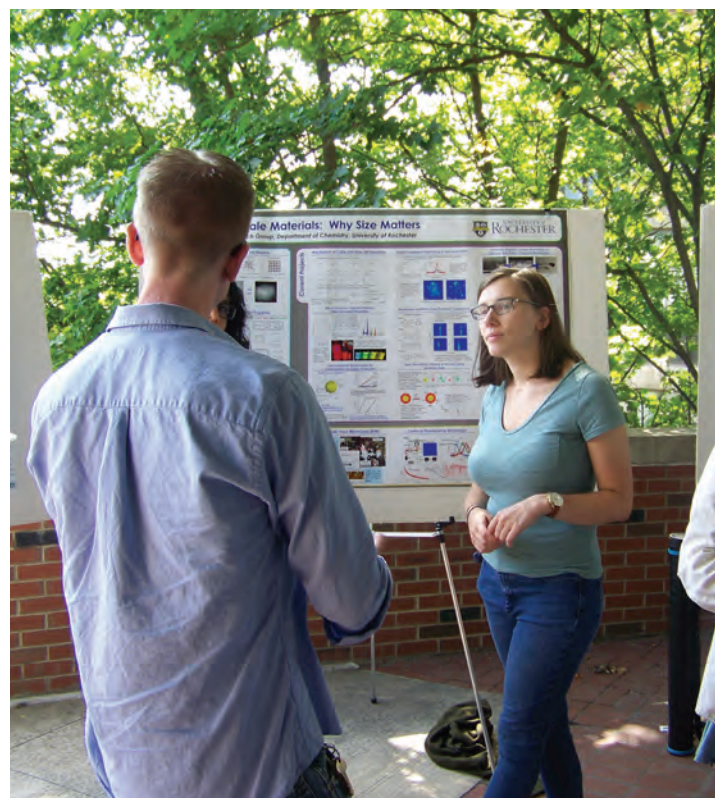
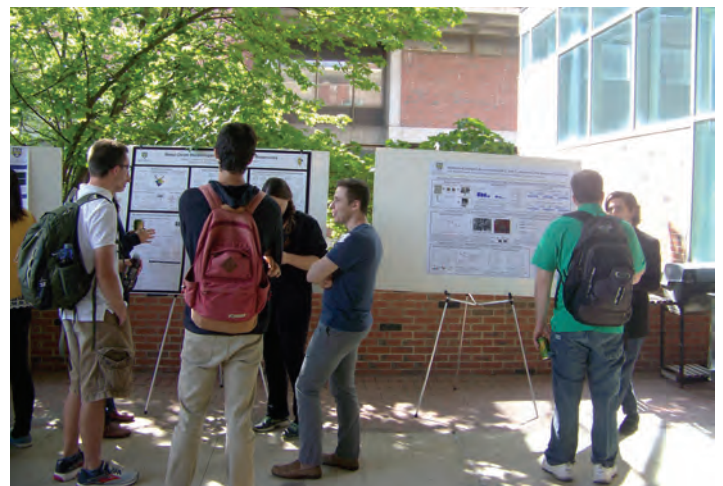
# Grad Student Welcome Party

On August 25th, 2017, the Chemistry Department finished up graduate student orientation week with a social hour and poster session, held on the porch of Carlson Library. It was a wonderful way to celebrate the start of a new year and to welcome our first-year students to the department!





# Grad Student Welcome Party





## 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

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During 2017, **ROBERT K. BOECKMAN, JR.** continued to teach full time and conduct research, while also serving as President and Chair of the Board of Directors of Organic Syntheses, Inc.

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 catalytic asymmetric spiroannulation chemistry has been developed and

application of this chemistry to a 2nd generation scalable synthesis 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 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**



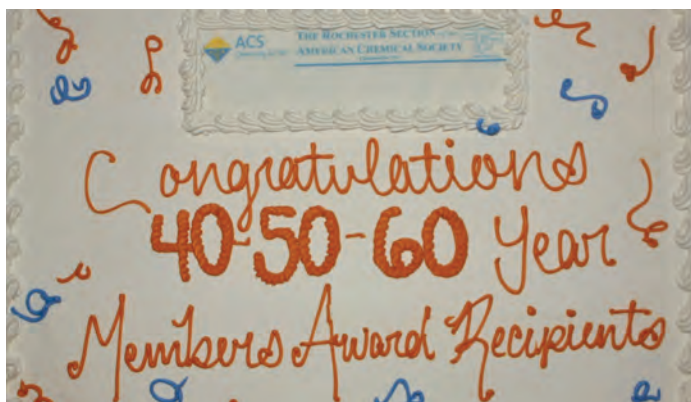
L to R: Venkat Srinivasan, Thomas Lyon (REU), Kyle Rugg, Don Batesky, Bob Boeckman, Justin Niziol, Noah Sims (REU), Dennis Savage



**WALDMANN.** Collaborations continue with **DR. HAL EBETINO (PH.D.'84)** (Research Professor in Chemistry), and with **DRS. BRENDAN BOYCE** and **LIANPING XING** of the URMCC Department of Pathology and Laboratory Medicine. These have resulted in the development of a Bone Targeted Drug Delivery Platform Technology including promising leads toward Bone Targeted Therapies for Bone Related Effects of Rheumatoid Arthritis, Osteoarthritis and Bone Cancer Chemotherapies. 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, is a temporary faculty member at RIT teaching laboratory courses. **LIFENG XIAO** defended his thesis in June 2017 and is currently a postdoctoral fellow at UC Berkeley working with Matt Francis. 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 URMCC. Fifth year student **KYLE RUGG** has nearly completed the 2nd generation synthesis of (-)-Nakadomarin A and will continue work toward Apoptolidin until his graduation at the end of 2018. Third 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. Part-time scientist **DR. DENNIS SAVAGE**, retired from Kodak, continues his work in the group on several projects. Recently, another Kodak retiree **DONALD BATESKY** has joined the group, and he will work on scale-up of intermediates for the targeted drug conjugate work as well as do some contract synthesis of liquid crystalline materials for a group at the Laboratory for Laser Energetics of the U of Rochester. The local Rochester section of the American Chemical Society honored 50, 60 and 70 year members at their awards and recognition dinner on Wednesday, October 11, 2017. Bob Boeckman and his wife, Dr. Mary Delton, were honored as 50-year members of the ACS. Shown below are each honoree with Dr. Allison Campbell, president of the ACS and research scientist from the Pacific Northwest National Laboratory.



*Bob's wife, Mary, receiving 50 year ACS award*



*Bob and Allison Campbell at ACS presentation* 37

# Kara L. Bren

Professor of Chemistry

Ph.D. 1996, California Institute of Technology



## RESEARCH INTERESTS

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

## CONTACT

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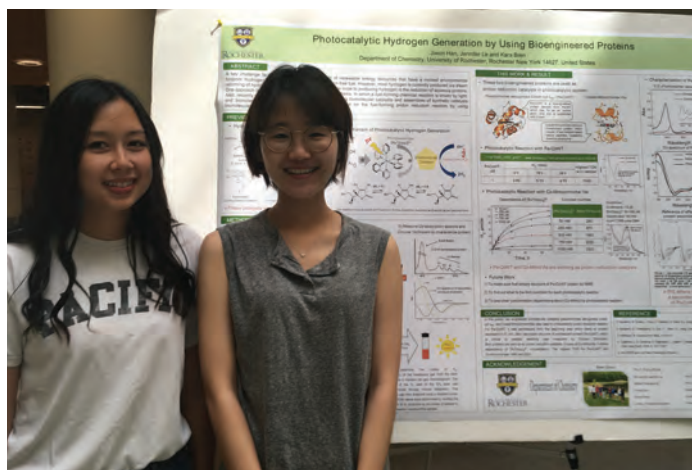
The Bren Group is continuing and expanding its work in the area of bioinorganic chemistry. A major emphasis of the group's efforts is the development of biomolecular catalysts for reactions relevant to energy and the environment.

The group wished a number of members the best as they took their next steps in their education and careers. Postdoc **PETER LAMBERG** moved to RIT to join the Schrlau lab where he is developing carbon nanotube array-based nanobiosensors for single cells. Graduate **BANU KANDEMIR (PH.D., '16)** completed her postdoctoral work at the University of North Carolina to move back to her original home of Cyprus, where she is now an Assistant Professor at the Middle East Technical University Northern Cyprus Campus. **LENORE KUBIE (PH.D. '14)** is moving from the Parkinson lab at the University of Wyoming to take a Postdoctoral position at the National Renewable Energy Lab in Golden, Colorado, with Matt Beard.

During the past year, the group was happy to welcome two international visitors. **VINCENZO FIRPO**, a Ph.D. student from Angela Lombardi's lab (University of Naples, Italy), spent over 1 year in the

group. Vincenzo introduced the lab to the Lombardi group's fully synthetic Mimochromes (mimics of cytochromes). During his stay, he developed these interesting biomolecules as catalysts for proton reduction. Vincenzo recently successfully defended his thesis. As part of the International REU Program, **JIWON HAN**, a Master's student from Ewha Women's University in Seoul, Korea, visited the lab during the summer to perform studies of photocatalytic hydrogen production.

Three new graduate students have joined the lab in 2016-2017. **JOSÉ LUIS ALVAREZ-HERNÁNDEZ** traveled from Havana, Cuba to spend the summer of 2016 with the group as part of the International REU program, and subsequently joined as a graduate student. Jose is performing electrochemical studies of cobalt porphyrin-based catalysts for hydrogen evolution. **JESSE STROKA** joined the group this past year as a second-year student and is focusing on catalysts for the reduction of nitrogen oxides. Finally, first-year graduate student **EMILY EDWARDS** recently joined the lab and plans to pursue studies of light-driven hydrogen evolution. The group also is happy to include two talented senior undergraduates, **CLAIRE DICKERSON** and **ALEX CALLAHAN**.



Jennifer Le and Jiwon Han





Claire is continuing work she started last year on electrocatalytic hydrogen production using cobalt metallopeptides. This year she is developing computational approaches to understanding mechanism in collaboration with Frank Huo's lab. Alex is working with Jen on engineering protein-based artificial hydrogenases.

Current graduate students on the lab are continuing their work on biomolecular catalysis. **SAIKAT CHAKRABORTY** has been leading the group's efforts in photochemical hydrogen production. In collaboration with Bechah Burke of the Krauss lab, he has developed a long-lived system for solar hydrogen production using a biomolecular catalyst. **JENNIFER LE** is engineering proteins for photochemical and electrochemical studies of hydrogen production. This work includes a collaboration with the Lombardi group. **YIXING GUO** has been a pioneer in the lab's work on metallopeptide electrocatalysts for both proton and nitrite reduction. As he wraps up his thesis work he is pursuing detailed mechanistic studies of these systems that have revealed interesting

and surprising effects. **SOMJIT BHAR** is working on related systems and has shown that changing the metallopeptide sequence alters reactivity, which provides an opportunity to understand and optimize catalyst structure and activity.

Kara enjoyed a busy 2017 with lots of visits to colleagues and friends all over the world. She was delighted to become a Kavli Fellow (National Academy of Sciences) and gave a lecture at Korean American Kavli Frontiers of Science Symposium at UC Irvine. Another highlight was an adventurous trip to Kolkata, India, to speak at the Symposium for Advanced Bioinorganic Chemistry. Kara particularly enjoyed the delicious food in Kolkata. She also was a Humphrey Lecturer at the University of Vermont, and traveled to Daegu and Seoul, Korea, to present at conferences (she was happy to reunite with Jiwon during this trip). In addition, Kara continued her work as an Associate Editor for JACS along with her Editorial Assistant Valerie Drake. Together they handled nearly 400 manuscripts during the year.



*The Bren Group (L to R): Kara Bren, Jennifer Le, Jose Alvarez-Hernandez, Jiwon Han, Somjit Bhar, Saikat Chakraborty, Alex Callahan, Jesse Stroka, Yixing Guo*



# Joseph P. Dinnocenzo

Professor of Chemistry

Ph.D. 1983, Cornell University



## RESEARCH INTERESTS

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

## CONTACT

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

Graduate student **ADAM FEINBERG** successfully defended his Ph.D. in January 2017. Among other things, Adam used nanosecond transient absorption spectroscopy to provide direct experimental evidence that alkoxy radicals can react with pyridine bases to give pyridinyl radicals. As far as we are aware, these are the first examples of alkoxy radicals acting as hydrogen atom donors in their reactions with a closed shell molecule. In addition, Adam also worked on the fragmentation chemistry aryltrialkyl Group 14 cation radicals. Adam discovered that like aryltrimethylstannane cation radicals (previously investigated in the group by **PU LUO(PH.D.'12)**, aryltrimethyl-silane and -germane cation radicals undergo fragmentation to give preferentially give the less stable aryl radicals rather than a methyl radical. Adam's work has provided important insight into the mechanism of these unusual reactions. Adam is currently enjoying a postdoctoral fellowship with Prof. Jeffrey Moore in the Beckman Institute at the University of Illinois at Urbana-Champaign. Joe

is looking forward to getting back together with both Adam and Pu at the upcoming National ACS meeting in New Orleans.

Third-year graduate student **ANALUZ MARK** is currently working to extend the research started by Adam and Pu on novel fragmentation reactions of Group 14 cation radicals, as well as continuing work on the reactions of alkoxy radicals as hydrogen atom donors.

Joe enjoys working in the lab on a regular basis. He and Samir Farid have been working on several projects involving novel exciplex intermediates. For example, they have discovered the first examples of charge-shift exciplexes formed between cationic, excited state electron acceptors and neutral donors. Interestingly, the electronic coupling between the donor and acceptors in the cationic exciplexes is even stronger than in conventional exciplexes, despite the lack of Coulombic attraction in cationic exciplexes. Joe and Samir, with help from Ana Mark, are currently exploring the scope and generality of these new exciplex intermediates.



*Aerial photograph of the University of Rochester (J. Adam Fenster)*



# Richard Eisenberg

Professor of Chemistry / Research Professor

Ph.D. 1967, Columbia University



## RESEARCH INTERESTS

Inorganic and organometallic chemistry; artificial photosynthesis and light-to-chemical 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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For **RICH EISENBERG**, the transition to a less research-active life continues. His current group consists of two postdoctoral students, **HONGJIN LV** (Ph.D. from Emory University) and **GUOCAN LI** (Ph.D. from Florida State University), with plans to close his lab in the first half of 2018 (both Hongjin and Guocan will have independent faculty positions by then). Fortunately, some of the equipment and facilities will remain for others to use as research on the photogeneration of hydrogen from water continues in other groups. For the last five years, Rich has collaborated as a co-Principal Investigator on two grants, one from DOE with Kara Bren as PI and Todd Krauss as another co-PI, and the second from NSF with Dave McCamant as PI. The two projects involve different aspects of the light-driven generation of hydrogen from water, which is the reductive side of water splitting for solar energy conversion into stored chemical potential energy.

The publications of the past year document continued progress in Rich's focus on solar hydrogen, including more effective light absorbers by coupling strongly absorbing organic dyes to charge-transfer metal complex chromophores for enhancement of photoinduced electron transfer, and new photocathodes having quantum dot absorbers of different sizes to promote electron-hole separation. Two of the publications were more personal retrospectives documenting a revisit to earlier Eisenberg chemistry.

Chemistry-related travels this past year included several meetings and celebrations. The first was at the Spring 2017 ACS Meeting in San Francisco where Rich gave several talks - one celebrated the 60th anniversary of the Division of Inorganic Chemistry and two were in recognition of friends (Marcetta Darensbourg and Bill Tolman) who received ACS national awards. In May, Rich travelled to Israel and the Weizmann Institute of



Rich and his wife, Marcia, on safari 41



*Eisenberg safari lion picture*

Science to participate in a special celebration for David Milstein who is another wonderful friend and was Rich's host when he was on sabbatical at the WIS in 1997. Rich also continued his activities as an Associate Editor of Proceedings of the National Academy of Sciences and a member of the Board of Chemical Sciences and Technology.

On the personal side were a hip replacement in June that went really well, a trip to South Carolina with Marcia, son Alan, daughter-in-law Shalla and the granddaughters

to see the solar eclipse, and a safari in Botswana with further travel to Cape Town, SA in September, 2017. The weather for the eclipse did not fully cooperate, but Alan did manage to get a great photo of the crescent sun (but clouds and humid air did preclude any vision of the corona). As for the safari, it fully lived up to its billing - the animals and photos of them were stunning - one safari friend is shown below. Rich is looking forward to a great 2018 with time in Sarasota increasing and a very special time at the New Orleans ACS meeting in March. One event will be a celebration of Cliff Kubiak's ACS Award in Organometallic Chemistry and another will be a celebration with long-time chemistry and NAS friends reaching the exalted age of 75.



*Eisenberg eclipse picture*

## Samir Farid

Research Professor

Ph.D. 1967, Göttingen University



### 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.

### CONTACT

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**SAMIR FARID** continues to collaborate with Joe Dinnocenzo on the dynamics of photoinduced electron transfer processes. The focus during 2017 was on two subjects: multiple exciplexes in highly polar media and a new class of exciplexes.

Whereas in low to moderate polarity solvents emission from a single exciplex is observed, in highly polar solvents the fluorescence spectra point to emissions from multiple exciplexes. In such polar solvents structures that increase the solvent stabilization start to compete with those that maximize the Coulombic interaction.

Over the last fifty years numerous examples of exciplexes have been reported. They all represent a charge transfer process (from neutral reactants to cationic/anionic pair), i.e., a charge formation reaction. The new class of exciplexes represents a charge shift reaction (from a cation/neutral pair to a neutral/cation pair) with no net change in charge. These charge shift (cationic) exciplexes broaden the scope and potential applicability in biological areas.





## RESEARCH INTERESTS

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

## CONTACT

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Imaging ion-molecule reactions is the theme for **JIM FARRAR**'s lab, but the past year has been one of transition.

During the Summer of 2017, Jim's Cornell colleague Floyd Davis took the time of flight mass spectrometer and two laser systems back to Ithaca. Jim took the first steps in dismantling and preparing the crossed beam imaging instrument for its move to Perugia, Italy, which he hopes to accomplish in June. He looks forward to many visits!

Jim was sad to learn of the death of his friend, Emeritus Professor of Biology Tom Bannister, on January 15, 2018. Tom was one of the first non-Chemistry faculty Jim met when he came to Rochester in 1976. Tom came to his office and asked "Are you related to the Farrars from Virginia?" Jim knew a little bit about his family history, and was aware that his ancestors had settled in Jamestown in 1618. He learned from Tom, whose ancestors were the Turpin family, that the Farrars and the Turpins owned adjacent plots of land on the James River. Tom told Jim about Farrar's Island in the James River, which the Farrar family owned for almost 100 years in the 17th and 18th century, and the two of them had hoped to walk the old land patents on the island together during the summer of 2017. Sadly, Tom's health failed quickly, and they were unable to make the

trip. Jim truly admired Tom not only for his interest in genealogy and his careful study of the many land patents along the James River, but also for his devotion to teaching and research at Rochester for many decades. Rest well, Tom!

Jim taught his last class in freshman chemistry in the Fall 2017 semester, rounding out 50 assignments in various versions of that course. To the many generations of students who have made teaching that course rewarding, Jim extends his grateful thanks.

Jim and Kathy continue to enjoy their roles as grandparents, without a doubt "the best gig in the world." Grandsons Callum and Cary in New York City, and granddaughter Josefina in Amherst, Massachusetts have been joined by baby boy Milo Martin, born November 30, 2016 to Mariana and Andy in Amherst. Jim and Kathy enjoyed several days on Cape Cod with all of them in August of 2017.



Prof. Tom Bannister and Farrar's Island plaque



Jim's grandchildren: Callum, Cary, Josefina, Milo Martin

# Rudi Fasan

Associate Professor of Chemistry

Ph.D. 2005, University of Zürich, Switzerland



## 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.

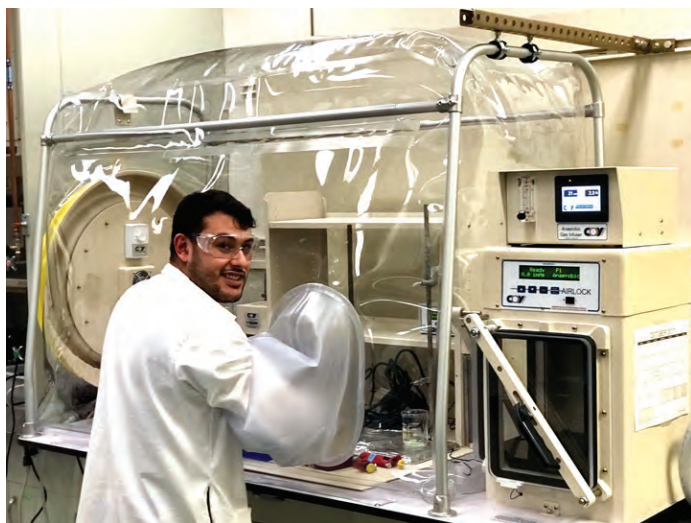
## CONTACT

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**PROF. RUDI FASAN** and his group continue their research focused on the development and application of new methodologies for the synthesis and evolution of macrocyclic peptide inhibitors of protein-protein interactions and on the design and investigation of metalloprotein catalysts for C-H functionalization and asymmetric synthesis. Over the past year, a major breakthrough in our peptide macrocycle projects was accomplished by fifth year graduate student **ANDREW OWENS** and postdoctoral fellow **IVAN DE PAOLA (POSTDOC, 2017)**, who developed a potent macrocyclic peptide inhibitor of the Hedgehog/Patched interaction, a key process implicated in the activation of the Hedgehog pathway (J. Am. Chem. Soc., 2016). This cell signaling pathway is misregulated in various types of cancer and this compound can now provide a tool for probing the therapeutic potential of this protein-protein interaction. This work was selected as a JACS Spotlight paper and it was also highlighted in Chemical & Engineering News, the magazine of the American Chemical Society. During the summer, Ivan left the group to take a scientist position at Fresenius-Kabi in Italy. This paper also featured former undergraduate student **YI-WEN (AMY) LIU**, who is currently completing a masters degree in chemical

engineering at Cornell University. Andrew brought to completion another project focused on the development of a high-throughput system for the directed evolution of aminoacyl-tRNA synthetases, which are useful enzymes for the incorporation of ‘non-natural’ amino acids into proteins (ChemBioChem, 2017). This project was realized with the assistance of former undergraduate students **KATHERINE GRASSO** and **CHRISTINE ZIEGLER**, who are currently graduate students at Boston College and Yale University, respectively.

Important progress was also made by the group members engaged in our biocatalysis projects. Fifth year graduate student **HANAN ALWASEEM** single-handedly completed a project related to the investigation of the anticancer activity profiles of a panel of semisynthetic parthenolide analogs obtained via late-stage P450-mediated C-H functionalization (Bioorg. Med. Chem., 2017). This work nicely demonstrated the value of our P450-based chemoenzymatic strategies for rapidly improving and modulating the pharmacological properties of a bioactive natural product. In collaboration with Gloria Saab-Rincon at the UNAM in Mexico, Hanan also reported the characterization of a panel of



David Vargas working in anaerobic chamber



Antonio Tinoco working in the lab



engineered P450 BM3 variants featuring a stabilized reductase domain generated via consensus mutagenesis (ChemBioChem, in press). Other members of the group have contributed to expand the reaction scope of engineered myoglobins as carbene transfer catalysts. In an impactful paper which appeared in JACS early this year, third year graduate students **ANTONIO TINOCO** and **VIKTORIA STECK** reported the development of a novel biocatalytic strategy for the asymmetric synthesis of trifluoromethyl-substituted cyclopropanes, which are highly valuable building blocks in medicinal chemistry. In addition to offering high enantioselectivity as well as stereodivergent selectivity, this method also features a clever two-compartment reaction setup for enabling the use of the gaseous (and toxic) carbene donor reagent trifluorodiazethane in combination with myoglobin-catalyzed cyclopropanation. To our delight, this work received highlights in both Chemical & Engineering News and Synfacts. In a collaborative effort with the computational group of Prof. Yong Zhang at the Stevens Institute of Technology, the same team has more recently completed a mechanistic study on hemoprotein- and iron-porphyrin catalyzed cyclopropanation. This work, which is to appear in the Journal of the American Chemical Society, contributed valuable insights into the mechanism of this reaction as well as a basis for rationalizing reactivity trends previously observed with this class of carbene transfer (bio)catalysts. In the meantime, postdoctoral fellow **GOPEEKRISHNAN ('GOPEE') SREENILAYAM (POSTDOC, 2017)** and third year graduate student **ERIC**

**MOORE**, along with Viktoria, spearheaded our efforts toward modulating and expanding the reactivity of these myoglobin-based biocatalysts through the incorporation of non-native metalloporphyrins cofactors (in place of the heme). In a first breakthrough in this direction, they were able to develop Mn- and Co-containing myoglobins capable of catalyzing the functionalization of C(sp<sup>3</sup>)-H bonds via carbene insertion, a reaction previously possible only using precious transition metals such as rhodium or iridium (Adv. Synth. Cat., 2017). In other exciting work, the same team developed 'green' (literally speaking) myoglobins which, by virtue of a non-native iron-chlorin cofactor, are capable of promoting the stereoselective cyclopropanation of olefins with diazo compounds with high efficiency under aerobic conditions (ACS Catal., 2017). Finally, Eric recently completed a project that introduces a novel and efficient strategy for enzyme stabilization via computationally guided 'protein stapling' (Proc. Natl. Acad. Sci. USA, 2017). This approach, which was implemented in collaboration with the Khare group at Rutgers University, combines state-of-the-art protein chemistry and protein design tools to achieve dramatic stabilization of a target enzyme against thermal and chemical denaturation, thus providing an attractive alternative to lengthy and laborious directed evolution protocols previously adopted for this purpose.

In addition to Ivan, this year the group bid a fond farewell to Gopee, who left the lab over the summer to take a tenure - track Assistant Professor position at Valdosta State



*The Fasan group at their Secret Santa party in December of 2017* 45

University, to postdoctoral fellow **PHUONG NGUYEN (POSTDOC, 2017)**, who took a staff scientist position at the URM across the street, and to undergraduate student **RACHEL BONN (B.S. '17)**, who graduated in May and is taking a year off to enjoy her newborn child prior to moving on to graduate school. The 'ranks' have been refilled with a cadre of talented and motivated postdocs, visiting scientists, and first year graduate students, who joined our group over the past twelve months. These include **DR. SACHITANAND MALI**, who came to our lab after receiving a Ph.D. from the IISER in Pune and postdoctoral training in peptide/protein chemistry in the Ashraf Brik lab at the Technion-Israel Institute of Technology, and **DR. AJAY CHANDGUDE**, who received a Ph.D. from the University of Groningen working on multicomponent reaction development in the Domling group. We also welcome visiting students **KRITTIKA RALHAN**, a Fulbright-Nehru research fellow from the Indian Institute of Technology at Gandhinagar, and **AGUSTINA VILA**, a UNESCO research fellow from the University of Uruguay in Montevideo. Last but not least, we were thrilled to make room in the lab for first-year graduate students **ANDREW BORTZ**, **YU GU**, **JACOB IANNUZZELLI**, **ALBERT NAM**, and **DAVID VARGAS**, who officially joined our group in December and have already begun to produce interesting results in their respective projects.

Throughout the year, our mid-career and senior graduate students have accumulated an impressive record of awards and accolades in recognition of their outstanding research accomplishments. These prizes include a Weissberger

fellowship to Andrew Owens, a Lattimore fellowship to **VIKTORIA STECK**, and a Hooker fellowship to **HANAN ALWASEEM**, who also received an Eli-Lilly Travel Award for participating and presenting her research at the ACS National Meeting in Washington, DC. **ANTONIO TINOCO** won one of the highly prestigious predoctoral fellowship from the Ford Foundation and his outstanding service as a teaching assistant was recognized by a Walters Teaching Award. Finally, **ERIC MOORE** was selected as one of the first trainees of the newly established T32 Training Program at the Chemistry-Biology Interface (CBI) funded by the NIH. We also celebrated the renewal of our NIH R01 grant, which will continue to support our research efforts in the area of metalloprotein catalysis and biocatalytic method development over the next four years.

Rudi continues to enjoy communicating the research achievements of his students and coworkers at invited talks at universities, companies, and conferences across the US and abroad. The highlights of the year have been two trips to the old continent to speak at the 13th International Symposium on Biocatalysis and Biotransformations and at the 20th International Conference on Cytochrome P450 in the beautiful cities of Budapest and Dusseldorf, respectively. At home, he enjoys spending time and relaxing with his wife Francesca, who keeps making new artistic creations with paper jewelry, his daughter Penelope, who is now a proud kindergartener, and his son Matteo, who keeps everybody entertained (and very busy).



*Antonio Tinoco received the Walters Teaching Award*



# Ignacio Franco

Assistant Professor of Chemistry

Ph.D. 2007, University of Toronto



## RESEARCH INTERESTS

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

## CONTACT

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We are a computational and theoretical physical chemistry group with broad interests in dynamical processes occurring at the nanoscale. We are particularly interested in developing new methods to probe and control the behavior of matter by means of external stimuli, a topic that we like to refer to as “Molecules Under Stress”. Research in our group is interdisciplinary in nature, typically at the interface between Chemistry, Physics, and Nanoscience.

During our first four years in Rochester we have worked on several fundamental problems in quantum mechanics as it applies to Chemistry, and developed strategies to bring theory closer to experiments that study the behavior of molecules in the presence of external bias voltages, mechanical forces and/or strong

laser fields. We use these insights to develop novel highly discriminating multidimensional spectroscopies that operate at the single-molecule limit, to understand the behavior of matter when driven far away from thermodynamic equilibrium, and to propose new ways to manipulate the behavior of matter. The group has been recognized by a NSF CAREER award and, more recently, by the ACS OpenEye Outstanding Junior Faculty Award in Computational Chemistry. This has been an exciting year for us, as some of the main papers of the group that we have worked on for several years are beginning to come out.

The group consists of six molecular “torturers”. The postdoctoral fellow, **DR. BING GU**, has made impressive progress understanding the physical processes that drive



The Franco Group (L to R): Bing Gu, Wenxiang Hu, Leopoldo Mejia, Antonio Garzon, Pawel Wojcik, James Savino, Zhi Li, Ignacio Franco

quantum decoherence in matter, constructing a theory for optical absorption of laser-dressed molecules, and developing a new method for quantum dynamics that offers favorable scaling of computational cost with system size. Because of his accomplishments, he received a travel award from the division of chemical physics to attend the APS March meeting in Los Angeles in 2018. Our senior Ph.D. student, **ZHI LI**, continues to make excellent progress understanding experiments that measure the conductance of a single molecule as it is mechanically manipulated. The third year Ph.D. students, **WENXIANG HU** and **ANTONIO GARZÓN**, have finished their first research project and are now writing their first few papers on electronic decoherence and Stark control of electrons, respectively. In addition, Antonio received his M.Sc. and is now a Ph.D candidate. Second year student, **LEOPOLDO MEJÍA**, has now completed his coursework and just submitted his first paper as part of the group investigating the information content of a class of electro-mechanical measurements in molecular junctions. Because of his accomplishments, he has been awarded a Sherman Clarke Fellowship. During the summer we had the fortune of hosting **PAWEL WÓJCIK** from the University of Warsaw as part of the highly prestigious international REU program of the Department. During his stay, Pawel investigated the absorption properties of laser-dressed materials.

The group has been very active in giving talks and presentations worldwide. Bing, Wen and Antonio presented their work in the Gordon Research Conference (GRC) on Quantum Control of Light Matter. Zhi and Bing presented posters in the “American Conference on Theoretical Chemistry” in Boston. This past year, Ignacio gave invited seminars at Purdue, Colorado State,

Erlangen and USC. He was also an invited speaker in “Congreso internacional de formación y modelación” (Medellín, Colombia), ACS MARM (Hershey, PA), “Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy” (Telluride, CO), “GRC on Quantum Control of Light Matter” (Hadley, MA), “Transport at the Nanoscale” (Cuernavaca, Mexico), “Charge carrier dynamics in nanostructures: optoelectronic and photo-simulated processes” (Bremen, Germany) and “Quantum Conductance and Forces across Molecular Junctions” (CUNY, NYC).

In terms of teaching, Ignacio keeps thinking of ways to enhance the understanding of Quantum Mechanics at a graduate and undergraduate level, and is currently redeveloping the graduate level course by incorporating active learning strategies. In addition to teaching, conducting research and writing grants, Ignacio was a member of a variety of committees at the University and beyond. This year, he served on the Graduate Recruiting Committee, the Colloquium/Distinguished Lectures & Seminars committee, the Faculty Club Subcommittee of the Faculty Senate Executive Committee, the executive committee of the Center for Quantum Coherence and Quantum Optics, and the Board of Directors of the Newman School. Ignacio also continues to lead and advance a Departmental program designed to bring top international undergraduate students to participate in research during the summer in Rochester. Ignacio was also involved in the hosting of Prof. Paul Brumer (Toronto) as the inaugural Clark Carroll lecturer of the Center for Coherence and Quantum Optics.

We look forward to a successful new year of research, teaching and service.





# Alison J. Frontier

Professor of Chemistry

Ph.D. 1999, Columbia University



## 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 love/hate relationship with divinyl ketones has led us to abandon them in favor of different types of pentadienyl cation precursors. For example, **PATRICK HARRINGTON** (5th year student) is studying cyclization cascades of dienyl diketones, a reaction that was first observed in 2005 by **PATRICK CARUANA (PH.D., '07)**. In the same vein, **GEORGE ALACHOUZOS** (3rd year) has discovered a novel, convenient way to access halopentadienyl cation intermediates by combining an enyne, an aldehyde or ketone, and a halide ion. These cyclize to deliver halocyclopentenes after stereospecific Nazarov cyclization. **ERIC STOUTENBERG** (5th year) is working to devise a new, improved synthetic strategy for the synthesis of tetrapetalone A. **DYLAN PARSONS** (4th year) and **SHUKREE ABDUL-RASHED** (2nd year) are each working to develop an unusual cationic cascade cyclization reaction.

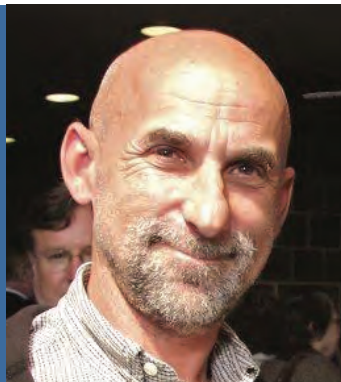
This year, we welcome **CONNOR HOLT** (BS Mercer University) to the group. We have four undergraduate colleagues working in the lab: **ILAN GOLDBERG** (class of '18), **CULLEN WALSH** (class of '19), **ALISON STANKO** (class of '19) and **PAUL SINCLAIR** (class of '20). Over the summer, we hosted **JAKUB VAITH**, an undergraduate from Imperial College (London) through the departmental international REU program. In the photo, you can see all of us (as well as my sons Danny and Connor) after spending three hours climbing around in trees at the Bristol Mountain Aerial Adventure Park.



## Joshua L. Goodman

Professor of Chemistry

Ph.D. 1984, Yale University



### RESEARCH INTERESTS

Organic chemistry: use of two complementary techniques, nanosecond laser flash absorption spectroscopy and pulsed time-resolved photoacoustic calorimetry to observe transient reaction intermediates produced following an initial photochemical event.

### CONTACT

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**JOSH GOODMAN** is currently serving as the Chair of the Undergraduate Studies Committee. His research interests are focused on the investigation of organic reaction mechanisms using a variety of time-resolved techniques such as pico- and nanosecond absorption spectroscopy, and photoacoustic calorimetry. In particular, he has been examining processes in which electron transfer is coupled to bond breaking, and/or bond making.

## Pengfei (Frank) Huo

Assistant Professor of Chemistry

Ph.D. 2011, Boston University



### RESEARCH INTERESTS

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

### CONTACT

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The **HUO** group develops and applies new theoretical approaches to investigate complex reaction dynamics, with a particular focus on photoinduced charge transfer and proton-coupled electron transfer reactions. This year is our group's first *Annus mirabilis*, with various exciting news including several publications and numerous awards for group members.

**DR. FARNAZ SHAKIB** has worked on developing new theoretical approaches that can accurately describe photochemical reactions affected by nuclear quantum phenomena. This work has led to one of our publications in *J. Phys. Chem. Lett.* (DOI: 10.1021/acs.jpcllett.7b01343), and has won her the highly competitive ACS Wiley Computers in Chemistry Outstanding Postdoc Award (as one of the two winners in 2018). With these impressive achievements, we wish her the best for her upcoming interviews for faculty positions.

**DR. SHARMA YAMIJILA** has finished up his two years of “quantum dynamics adventures” in our group and is heading to UC Riverside for his next postdoc position. Sharma has worked on developing new computational methods that can accurately simulate photoinduced charge transfer in organic photovoltaics. These new results will appear soon in a just submitted paper to *J. Chem. Theory Comput.*, as well as numerous following publications. We wish Sharma and his family a nice and lovely stay in warm southern California and look forward to future scientific collaborations.

**SUTIRTHA CHOWDHURY** made his first breakthrough in his graduate career. He has developed a new theoretical approach that can provide a unified description for electron and proton transfer. This new theoretical approach, coherent-state ring polymer





*The Huo Group (Front Row): Xinyang Li, Pengfei (Frank) Huo, YSKRC Sharma, Sutirtha Chowdhury, Arkajit Mandal (Back Row): Juan Sebastian, Farnaz Shakib*

molecular dynamics method is publication in *J. Chem. Phys.* (doi.org/10.1063/1.4995616). With his excellent research and teaching services, Sutirtha won a Sherman-Clark fellowship and W.D. Walters Teaching Award this year.

**XINYANG LI** continues his exciting project of using ab-initio quantum dynamics to simulate kinetic isotope effects in proton transfer reactions. Some of his recent results are currently being considered for publication. Joining forces with Sutirtha, Xinyang will use new theoretical approaches to uncover the complex mechanism of proton-coupled electron transfer reactions. Xinyang is also actively collaborating with the Bren group on exploring hydrogen evolution reaction, helping other graduate students in the department to perform electronic structure calculations, and becoming the “theory gadget wizard” in the department.

**ARKAJIT MANDAL** has placed himself in a very competitive position as a successful future theoretician. With a wonderful idea so-called quasi-diabatic representation, he and Sharma worked collaboratively and resolved a long-lasting challenge in theoretical chemistry: the incompatibility between electronic structure methods and quantum dynamics approaches due to their different “footing”. This work was submitted to *J. Chem. Theory Comput.* for publication. Arkajit also won a Sherman-Clark fellowship because of his excellent academic and research achievements.

**SEBASTIAN SANDOVAL** has begun his quantum

dynamics journey in our group, working on several new non-adiabatic dynamics simulation techniques where electronic states can jump from one to another upon excitations.

This year, we have two undergraduate students, **RACHEL CLUNE** ('18, winner of Catherine Block and Junior Scholar Award) and **ZACHARY MARSHALL-CARTER** ('19) in our group for their senior research. In the summer, we also hosted three additional undergraduate researchers in the group, **YOSHIMI ARAKI (REU, '20)**, **MATTHEW AQUILINA (REU, '19)**, and **ALESSANDRO ROGNONI (I-REU, U OF MILAN)** performing quantum dynamics simulations. **MARIA CASTELLANOS**, a former i-REU student, continues working with us throughout this year; her work on singlet fission has been published in *J. Phys. Chem. Lett.* (DOI: 10.1021/acs.jpcclett.7b00972).

The group has actively traveled and presented these new and exciting results over the past year. Frank gave four talks at the ACS meeting at San Francisco and was invited to talk in the “singlet fission workshop” organized by Prof. Josef Michl. He also participated at the American Conference on Theoretical Chemistry in Boston this year. Farnaz presented her results in terms of two talks at ACS (Washington DC) and APS (New Orleans) meetings. Sebastian was selected to participate at the Telluride School in Theoretical Chemistry and presented a poster there. Farnaz, Arkajit, and Sutirtha also went to the Penn Conference in Theoretical Chemistry to present their results.

In addition to the exciting research activities and writing grants, Frank is also serving on the Graduate Recruiting and Graduate Studies committees. In summer, the Huo group conducted our first “Journey to the Molecular World” summer school for local high school students in the Rochester City School District. This course is designed as a brief introduction to Computational Chemistry and aims to inspire the curiosity and enthusiasm of the students about

molecular science. This year, Frank taught Statistical Mechanics (CHM 455) twice in a row, which is a rare event in statistics. Theory division is also honored to host Prof. David Beratan (Duke), Prof. Bill Miller (Berkeley), and Prof. Victor Batista (Yale) to give talks this year.

We plan to keep our momentum and looking forward to another *Annus mirabilis*.

## 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 one new member join the group this year, **ANDY VANDERWEIDE**, who will be working on our NSF funded research in heterocycle synthesis. **DR. NAVEEN KULKARNI** moved on to a new faculty position at Amrita University, in Kerala, India (<https://www.amrita.edu/faculty/naveenvkulkarni>). **MILES WILKLOW-MARNELL** finished his Ph.D. in July, and is now on the faculty at SUNY New Paltz. **LLOYD MUNJANJA** finished his Ph.D. and is now working at the Center for C-H Functionalization at Emory. The group had a visitor from the Univ. Paul Sabatier, Toulouse, France. Graduate student **MARION BEGUERIE** came and worked in the lab for several months in fall 2016.

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 we filed a patent on this discovery. The group just completed its participation in the Center for Enabling New Technologies through Catalysis (CENTC), a collaborative research effort that spanned the past 13 years and involved projects that explored electrophilic C-H activation catalysts, direct

routes to aniline from benzene, electrochemical bond activation, and the above mentioned butanol process. 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 Vanderbilt, University Cincinnati, Peking University, Tsinghua University, Osaka University, Keio University, University Rennes, University South Carolina, UC Riverside, UCLA, UCSD, UBC, Stony Brook, Fudan University, Tongji University, University Bristol, University of Galway, and University of York. He also spoke at the International Symposium on Organic Chemistry in Western China, Chengdu, China, and the Symposium on Nickel and Related Chemistry, Shanghai University, Shanghai, China. He taught a short course on Aspects of Organometallic Chemistry at Kyoto University during January 2017, where he was a Distinguished Visiting Project Professor. Bill won the Royal Society of Chemistry Organometallic Chemistry Award for 2017 and received his award during a lecture tour in the U.K. He also just learned that he was awarded a Humboldt Fellowship for 2018 and will be moving to Berlin with Heather for a 6-month sabbatical at the Free University of Berlin with Prof. Dr. Christian Müller in January. Bill also did a podcast on WXXI Connections on “Carbon Capture, And How It Relates To Climate Change.”



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. 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  $\alpha,\beta$ -unsaturated aldehyde. Rehydrogenation gives butanol, with water as the only byproduct. We have found a very selective tandem catalyst system that give only n-butanol but no higher Guerbet products (products resulting from butanol reacting in a similar fashion with itself or with ethanol).

As mentioned above, our work in a collaborative research effort in the Center for Enabling New Technologies through Catalysis (CENTC) ended this

year. This NSF-funded center included researchers from a dozen universities participating in joint projects and using cyber-conferencing to discuss results. This mode of research tested a new paradigm for conducting collaborative research and finished after 13 years of funding. Our group has completed several collaborative projects with the Goldberg group, the Goldman group, the Mayer group, the Miller group, The Baker group, and the Cundari group through CENTC. Bill will serve on the International Advisory Board for the ICOMC and ISCHA conferences. The group is supported by continuing funding from the Department of Energy and the National Science Foundation.

Bill's grandson, Henry William Simson, born to his daughter Sarah and her husband Michael, is now 3 years old. Henry is 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.





# Kathryn Knowles

Assistant Professor of Chemistry

Ph.D. 2013, Northwestern University



## RESEARCH INTERESTS

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

## CONTACT

kknowles@ur.rochester.edu

This past year has seen a tremendous amount of growth for the **KNOWLES** group in both personnel and lab space. After spending the fall of 2016 doing experiments in two hoods borrowed from the Krauss group on the second floor of Hutchison Hall (thanks Krauss group!), Katie and her first graduate student, **MEHRIN TARIQ**, made way for lab renovations by moving upstairs to a fourth-floor lab borrowed from the Rothberg group (thanks Rothberg group!). They were joined by two new graduate students, **JORDAN ANDREWS** and **DAVID BREWSTER**, and three undergraduates, **DOMINICK SARAPPA ('18)**, **TAE RYOO ('18)**, and **JOSHUA LOMELO ('18)**. While in this temporary lab space during the spring semester of 2017, the group made progress on initial projects focused on the synthesis of copper and iron oxide nanocrystals.

Dom and Josh continued their research as part of the summer REU program, and we also had the pleasure of hosting an international REU student, **ANA CLAUDIA FINGOLO**, who joined us from Brazil. July was probably the most eventful month for the group this year: Mehrin passed her qualifying exam, Katie and David worked with colleagues Prof. Dave McCamant and Mike Mark to co-teach a summer mini-course about solar energy as part of the Upward Bound program, and the group moved into beautifully renovated lab space on the second floor of Hutchison Hall where the Center for Photoinduced Charge Transfer used to be located. The excitement of setting up the new lab will culminate in 2018 with the installation of our new femtosecond amplified Ti:Sapphire laser system. This final piece of equipment will enable us to use transient absorption spectroscopy to study the dynamics of photogenerated charge carriers in metal oxide nanomaterials.

Overall it has been an exciting year for the Knowles group and we look forward to a productive 2018. Stay tuned!



(L to R): Tae Ryoo, Mehrin Tariq, David Brewster, Kathryn Knowles, Jordan Andrews, Joshua Lomeo, Dominick Sarappa



# Todd D. Krauss

Professor of Chemistry

Ph.D. 1998, Cornell University



## RESEARCH INTERESTS

Physical chemistry; synthesis and characterization of nanometer scale materials and devices with relevance for renewable energy, techniques include single molecule photoluminescence spectroscopy, atomic force microscopy, ultrafast and nonlinear optical spectroscopy. Biophysical chemistry; single molecule studies of protein folding structure and dynamics.

## CONTACT

krauss@chem.rochester.edu

More **KRAUSS** group REAL news from 2017:

**NICOLE M. B. COGAN** is still studying how to make a molecule with truly amazing photophysical properties including the ability to emit “quantum light” continuously. In fact, while we still don’t know what the molecule structure is.... Nicole has found no less than five different ways to “make” it! Working closely with Alison Frontier’s laboratory, we hope to identify the structure of the mysterious molecule shortly now that we can synthesize the molecule somewhat reproducibly. Nicole is gunning for “molecule of the year” for her discovery. **ZHENTAO HOU** published her first paper as a

primary author in 2017. Congrats! She is building off that work and is studying the effect of photoluminescence brightening agents on individual nanotubes that are longer than the diffraction limit, with the hope that the longer nanotubes will enable a greater understanding of this interesting process.

When not riding the mechanical bull in NOLA, **AMANDA AMORI** is working on refining her understanding the photophysical dynamics of intervalley scattering of excitons in carbon nanotubes with Zhentao. In fact Amanda’s first paper on this subject should be published in early 2018 – congrats Amanda! Amanda is also working on some really hard measurements of trion photophysics in single nanotubes at low temperature that we hope to report on sometime in 2018 as well. This past summer “world traveler” **LEAH FRENETTE** added another country to her resume: Sri Lanka. Despite being on a plane a lot, she published two papers in 2017. Her first paper was co-authored with Kelly Sowers (currently in the Netherlands doing a postdoc at Utrecht University) on photoredox catalysis in collaboration with Jill Caputo and Dan Weix. Leah’s second paper came out in December and focused on the reaction mechanism behind the synthesis of CdSe and like quantum dots, whereby she solved a puzzle that was over 30 years in the making!

**ABBY FREYER** made major breakthroughs in trying to understand what happens when CdSe quantum dots are doped with silver ions. She observed a strong relationship between the photoluminescence and the average charge properties of the doped quantum dots using electrostatic force microscopy, which she found is surprisingly due to exposure of the dots to ions and has nothing to do with actually doping the dot per se. Working with researchers at Cornell University, Abby also used fancy electron microscopy techniques to locate the silver atoms in the CdSe particles.... and she found that the quantum dots



The Krauss group at a hockey game



are extremely heterogeneously doped with most of the silver located in a few large particles of silver selenide. I suspect these two findings will create quite a stir in the doped quantum dot community!

**JENNIFER URBAN**, our first joint **NILSSON-KRAUSS** student has gotten her TIRF setup working over here in the Krauss lab, and is making great progress in assessing whether quantum dots can outperform dyes for super-resolution imaging purposes. Jen is also working with Dr. Harry Stern to apply more advanced computational data analysis techniques to the super-resolution data to create more accurate sub-diffraction limit images. **BECKAH BURKE** has made some big breakthroughs on her project as well. Working in collaboration with the laboratory of Kara Bren, Beckah found that combining glutathione capped quantum dots and bio-inspired, cobalt catalysts created an excellent integrated system for photochemical proton reduction to hydrogen. What is exciting is that this system seems to work as well as our original Ni catalyst system from over 6 years ago, although we don't quite understand why. Beckah is working on the "why" now and hopes to publish an article on her findings early in 2018.

I want to give a shout out to some new members of the group who joined in late 2016. **JIAJIA YIN** is a visiting student from China who won a prestigious scholarship to study in the U.S. for two years. She has synthesized excellent quality CdTe quantum dots and is testing their performance for photocatalytic proton reduction with small molecule nickel catalysts. Sean O'Neill is a second year Materials Science student who is working on the synthesis and photophysical characterization of

SnTe quantum dots. These particles should be direct gap semiconductors in the infrared (we think) and may have some interesting topological charge transport properties.

Finally – we want to welcome brand new group members **MAHILET HAILEMICHAEL** and **TREVOR TUMIEL!** Mahilet is a first year Materials Science student and is going to work on the solar fuels project in collaboration with Kara Bren's and Ellen Matson's labs. Trevor is a first year Chemistry student and is excited about studying single-walled carbon nanotube photophysics. During the summer of 2017 the group (well really Abby) hosted an ACS Project SEED student Karina Le. Karina had a great time doing "real" science and we got to learn from her what all the cool kids are doing in High School these days!

In other news, due to the lab renovations for Katie Knowles, we had to do a little bit of space shuffling on the second floor and as a result the wet-lab was completely renovated. It looks fantastic and, more importantly, the group is really enjoying the better use of wet space and especially the 8-foot hoods! Note that there is a rumor that photos of Amanda Preske's latest line of jewelry from her company Circuit Breaker Labs may be involved in the background of some cool looking lab space as well....

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! <https://www.facebook.com/groups/kraussgroup/>



*The Krauss group at the Lilac Festival*



# Thomas R. Krugh

Professor of Chemistry

Ph.D. 1969, Pennsylvania State University



## 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

[krugh@chem.rochester.edu](mailto:krugh@chem.rochester.edu)

During the Spring 2017 semester, Tom's teaching was combined with organizing another summer Research Experience for Undergraduates (REU) program for summer. The 2017 REU program included a total of 33 students, with 7 students from other US institutions, 6 students supported by the Department's international REU program, and 20 University of Rochester students! Tom has directed our NSF funded REU program for the past 18 years, and he takes pride in organizing a program that includes a large number of UR students. For most Rochester participants, the summer REU program is their first full-time opportunity for research.

The Fall 2017 semester began the transition towards retirement at the end of the 2017-2018 academic year. Tom has always considered it an honor, and pleasure, in helping the 300 students in his section of Chemistry 131 learn and enjoy the material (as much as possible in a challenging class). The nineteen workshop leaders that are critical to student learning create another opportunity of responsibility in teaching a large class, but also provide pleasure in helping these young scholars earn student comments such as "My workshop leader was fantastic." Tom even values the comment "I learned so much more in workshop than in lecture" because true learning is best facilitated by active engagement/review of material.

On the personal side, Tom and Rody continue to enjoy traveling, especially to visit with their son Brad, his wife Charlotte, and our two granddaughters, Julia (9) and Eliza (7). A photo from a family wedding in Boca Raton, Florida in June 2017 is included. Brad and Charlotte live in Wilson, Wyoming, although recently have been spending time in Seville, Spain. Tom and Rody had an enjoyable fall break trip to visit with them.



*Tom Krugh family picture*



## RESEARCH INTERESTS

The push to generate electricity from renewable sources has created a 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 catalysis and energy storage.

**CONTACT:** [matson@chem.rochester.edu](mailto:matson@chem.rochester.edu)

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 cluster complexes. As recognition for our creativity and truly impressive preliminary results, the Matson Group was awarded their first major grant, an NSF CAREER Award!! We will be using the funds to continue our research focused on the synthesis and reactivity of iron-functionalized polyoxovanadate-clusters.

In January, **SAMUEL WEINSTEIN** (SUNY Geneseo) joined the team. He is currently working on the synthesis and reactivity of iron-functionalized polyoxovanadate-alkoxide clusters, picking up where our postdoc, **FENG LI**, left off. Sam is making great strides toward the development of high-yielding, efficient routes to access the cluster. We plan to translate his results into a laboratory for undergraduate students this Summer. In late July, **FENG** and his family headed out to San Francisco, where he now works for the chemical company Air Liquide. We wish him success in his future career!!

Some major group milestones: **RACHEL MEYER**, **BRITTNEY PETEL**, and **LAUREN VANGELDER** passed their oral exams and advanced to Ph.D. candidacy! They continue to make great strides toward their research goals, each working toward first-author publications that will be submitted in early 2018.

The graduate students in the Matson Group continue to work extremely hard to make an impact in both the department and community. The group attended multiple conferences, namely the Western New York Inorganic Symposium, held at Cornell University in June, and the Inorganic Discussion Weekend in Toronto, Canada. Additionally, the lab took part in the Teacher's Challenge

5K to raise money and show support for teachers in the Rochester City School District. This athletic accomplishment is part of an ongoing effort in the Matson Lab to connect with the Rochester Community. In the Fall of 2017, **BRITTNEY PETEL** served as an instructor for a brand-new course in the College of Arts and Science, entitled CAS 207: Chemistry Engagements in the Rochester City School District. In this course, Brittney led a team of undergraduate students in developing curriculum for classroom visits during National Chemistry Week. The event was executed perfectly, and the financial support from the University of Rochester's Center for Community Leadership allowed for the expansion of the program to include 30 classrooms, reaching 650 students. Major thanks to all in the department and university community who volunteered to lead lessons!! Special thanks to Brittney for bringing a whole new dimension to this event!

Additionally, the group was fortunate to be recognized with a variety of awards and honors this past year. **LAUREN VANGELDER** was named a recipient of the prestigious National Science Foundation Graduate Research Fellowship, and also won first prize for her poster at the New York Battery and Energy Storage Technology Consortium. Lauren was also the winner of



*Ellen Matson with husband Scott and baby Tad*



the Laura & Elliot Richman Travel Award; she will be traveling to her first Gordon Conference this Summer. **BRITTNEY PETEL** was awarded the Samuel Allen and Ellen Frances Lattimore Graduate Fellowship! Ellen was selected to present the group's exciting results in a prestigious poster talk at the Inorganic Reaction Mechanisms Gordon Conference. Ellen was also named a recipient of the University of Rochester's Valerie and Frank Furth Fund Award in recognition of her accomplishments during her first two years as a faculty member.

Undergraduate research in the Matson laboratory has continued to thrive. This Summer, we welcomed **IAN BRODKA ('18)** and **PATRICK FORRESTREL ('18)** to the team as a part of the University of Rochester REU program. This Fall, **ROBERT SCAPPATICCI ('18)** came on board, helping to put the finishing touches on manuscript describing our group's efforts in cross-coupling catalysis (a new area of research for our laboratory). **MERJEMA PURAK ('17)** has continued her work in the Matson Group. In recognition of her excellence, she was awarded both the Catherine Block Memorial Prize and the Junior Scholar Award. Anticipating her departure to graduate school this summer is a bit too much for the group to bear, but we are excited to see where she takes her talent next!

We've also had the privilege of welcoming an international exchange student into the laboratory for the 2017-2018 academic year. **LOUISE BYRNE ('18)** is an undergraduate student from Bristol majoring in Chemistry. As a part of her degree, Louise is spending a year in Rochester taking classes and performing research.

Ellen spent 2017 talking, travelling, and teaching. In addition to attending the Inorganic Reaction Mechanisms Conference in March, she also travelled to San Francisco for the Spring ACS meeting, where she was invited to participate in a symposium entitled "Sustainability in Electrocatalytic Fuel and Chemical Production". Over the Summer, Ellen traveled to Washington D.C. to serve as a facilitator for the ACS Postdoc to Faculty Workshop, helping aspiring faculty compile application materials and prepare for a career in academia. At the University of Rochester, in the Spring of 2017, Ellen taught a brand-new graduate course focused on fundamental Small Molecule Activation. The course received great reviews and will be continued in the Spring of 2018. This Fall, Ellen started teaching the introductory inorganic chemistry course (CHM 211). She has absolutely loved getting to spend more time with undergraduate students!

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 2018 has in store!



*The Matson Group (L to R): Lauren VanGelder, Rachel Meyer, Ellen Matson, Brittney Petel, Sam Weinstein*

# David W. McCamant

Associate Professor of Chemistry

Ph.D. 2004, University of California, Berkeley



## RESEARCH INTERESTS

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

## CONTACT

mccamant@chem.rochester.edu

The **MCCAMANT** group has had a fun year filled with science and spectroscopy. **DAVE** used the spring to develop new lab modules to teach in CHM231 in the fall. That class now has exciting new experiments studying dissolved lead in potable water in Rochester and dye-sensitized solar cells for solar energy harvesting. Graduate students **MIKE MARK** and **ZAK PIONTKOWSKI** were joined by first-year graduate student **STEVEN DIAZ**, who matriculated in the fall of 2017. Steven came to us from the University of Northern Colorado where he did a lot of work on metal nanoparticles. Now we just need him to get those nanoparticles to make some hydrogen!

**MIKE'S** work has focused on the ultrafast dynamics of rhodamine-like dyes in aggregates and on TiO<sub>2</sub> surfaces probed with transient absorption. He's developed skills to make samples of aggregated dyes that maintain transparency in solution so that we can probe the extraordinarily weird dynamics of the H-aggregated excitons. Cool stuff! Mike has also been working hard on collaborations with **GUOCAN LI**, postdoc in the Eisenberg group, to probe energy transfer dynamics in rhodamine-PtN<sub>2</sub>S<sub>2</sub> compounds and with **DR. CHRIS COLLISON (POSTDOC, ROTHBERG GROUP, '96-**

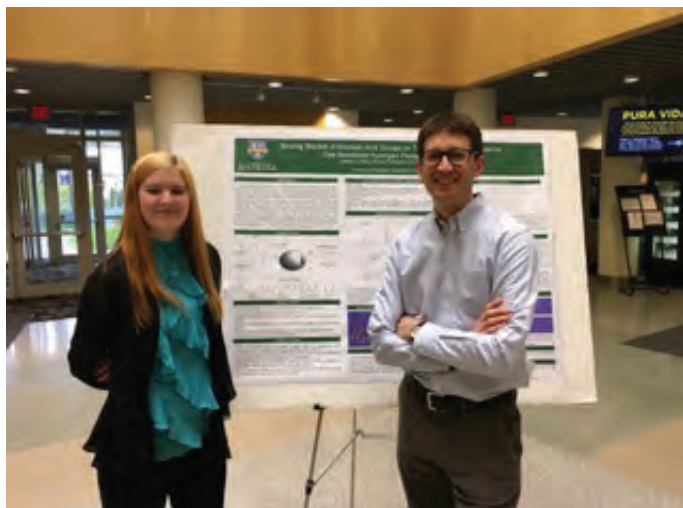
**'99)** at RIT, to probe energy transfer dynamics in squaraine dyes used for organic photovoltaics.

**ZAK** has completely rewritten the code for calculating resonance Raman excitation profiles (Goodbye, Fortran 77!) and has used it to determine the structural changes in rhodamine dyes upon absorption of light. His experimental and theoretical studies of the dyes synthesized in the Detty lab at SUNY Buffalo have provided the best insight to date on the structural dynamics of the excited monomeric dyes in solution. Zak also spearheaded a collaboration with **RANDY SABATINI (P.H.D., '15)** in the Sargent lab at the University of Toronto to study the CW Raman spectrum of lead-halid perovskites used for novel photovoltaics and OLEDs. (Randy has now finished his appointment in Toronto and moved to second postdoctoral position studying photoactive nanomaterials in Australia.)

Visiting graduate student, **ZHI WU**, from Xiamen University in China has been working with us throughout 2017 and will continue in 2018. Zhi has used her background in nanomaterials synthesis to develop new methods to synthesize strontium titanate nanocrystals.



Prof. McCamant at ACS award dinner



Jessica Freeze with Prof. McCamant at senior poster session



That's right, we are doing some synthesis in the lab now! (Though with very little advice from Dave.) Recently, Zhi has been using femtosecond transient absorption to better understand the heterogeneous electron transfer dynamics of PtN<sub>2</sub>S<sub>2</sub> chromophores into TiO<sub>2</sub> nanoparticles.

In the spring of 2017, **JESSICA FREEZE (B.S. '17)** continued her work on the mechanism of binding of aromatic phosphonates onto TiO<sub>2</sub> nanoparticle surfaces. Jessica performed electronic structure and dynamics calculations on these systems that explored

the rapid electron transfer from the molecular LUMO to the nanoparticle conduction band. Jessica is currently enrolled in the chemistry doctoral program at Yale University. This same system was explored over the summer when **MELISSA MARX** joined our lab, on loan from Alfred University through the REU program. Melissa collected excellent CW Raman spectra that showed, experimentally, many of the features that Jessica first highlighted in her simulations. Of course, Zak provided extraordinary mentorship throughout both of these projects.

## Michael Neidig

Assistant Professor of Chemistry

Ph.D. 2007, Stanford University



### 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 has had a very exciting year in non-precious metal catalysis and f-element chemistry. The group currently consists of seven Ph.D. students and two postdoctoral scholars, with **NIKKI WOLFORD** (Millersville) and **DAN CURRAN** (College of New Jersey) joining the group last year as new Ph.D. students and **DR. PETER NEATE** (Ph.D. University of Edinburgh) joining as a postdoctoral scholar. The group also said goodbye to the last original member of the team from the very beginning when **DR. JARED KNEEBONE** successfully defended his Ph.D. this past July. Jared is currently a postdoctoral scholar with Prof. Andy Borovik (UC-Irvine), and we wish him the best struggling through winters on the West Coast.

The group had another highly successful research year, with publications spanning projects in iron-catalyzed cross-coupling, metals in biology, f-element chemistry and iron-based ORR catalysts in fuel cells. Of particular note was a huge study determining the mechanism of iron-SciOPP cross-coupling with alkynyl nucleophiles as well as the first f-element publication from the group investigating the application of magnetic circular dichroism spectroscopy to coordination complexes of uranium. The group's research success is all due to

the excellent student and postdoctoral researchers in the group, many of whom were individually honored this past year. **VALERIE FLEISCHAUER** received the inaugural Outstanding Graduate Student Award from the department at the end of 2016, and both she and **STEPHANIE CARPENTER** were recipients of prestigious Elon Huntington Hooker fellowships from the University of Rochester. Many students also received travel awards to support the presentation of their work at the ACS National Meeting in Washington, D.C. in August, including **STEPHANIE CARPENTER** (ACS Division of Inorganic Chemistry travel award), **VALERIE FLEISCHAUER** and **TESSA BAKER** (Department travel awards and Graduate Women in Science travel awards). Lastly, Stephanie was also a finalist for Three Minute Thesis Competition at the university this past year. We were all very excited to come out and support Stephanie as she endeavored to summarize her Ph.D. project in three minutes (for a non-scientific audience!). Last but certainly not least, **STEPHANIE CARPENTER** was also recognized with a poster award at this past year's Western New York Inorganic Symposium held at Cornell University.



*Neidig Group*

The group also once again hosted students from Monroe Community College and local high school students for summer research experiences. Also in the summer, Valerie and Tessa both got a taste of industrial research through summer internships with companies in the Rochester area. In November, the vast majority of the group also made our annual pilgrimage north for the 50th Inorganic Discussion Weekend which was held at Ryerson University in Toronto. Mike had several long distance trips this past year to spread the word

on the group's most recent chemistry, including talks at the ISACS (Manchester, U.K.), Gordon Inorganic Reaction Mechanism (Galveston, TX) and Gordon Organometallics (Newport, RI) conferences as well as a trip to Lomonosov Moscow State University. Last but certainly not least, Mike was excited to be promoted to Wilmot Associate Professor with tenure, enabling him to withdraw all of his pending Taco Bell employment applications. Moving forward, we anticipate another exciting year of research in non-precious metal catalysis and f-element chemistry at Rochester.



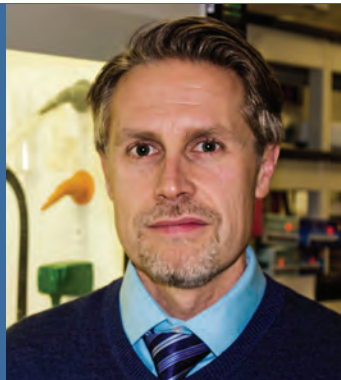
*Neidig Group at their 2017 holiday party*



# Bradley L. Nilsson

Associate Professor of Chemistry

Ph.D. 2003, University of Wisconsin, Madison



## RESEARCH INTERESTS

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

## CONTACT

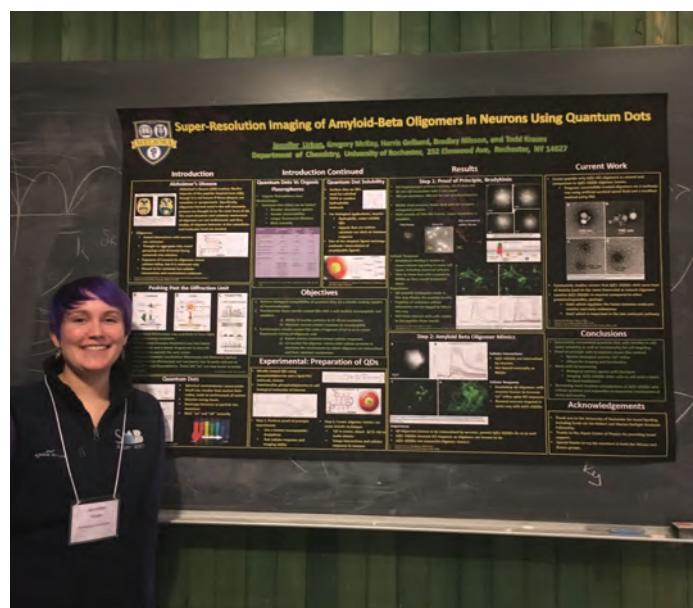
nilsson@chem.rochester.edu

The **NILSSON** group had a busy and productive year in 2017. Current and former graduate and undergraduate students are advancing their research projects and reaching significant professional and personal milestones. The group published seven peer-reviewed publications, submitted the final manuscript for a book volume, taught many classes as instructor or teaching assistants, had new research grants funded, and attended meetings all over the world (US, Canada, and India) in the last year. We're carrying this momentum forward in 2018 and look forward to more success as at least three of the Nilsson group's students prepare to complete their Ph.D. studies.

**DANIELLE (RAYMOND) RIEGLE** has made significant advances in her research projects and we expect that she will defend her Ph.D. thesis during the summer of 2018. Danielle is studying rippled  $\beta$ -sheet materials derived from the coassembly of enantiomeric peptides and is seeking to apply these materials to novel applications as HIV microbicides and as hydrogels for tissue engineering. She also 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. The project has had an excellent start and we're very excited about the potential of this new research direction for our group. Danielle received a travel grant to attend the 25th American Peptide Symposium in Whistler, BC, Canada in June. She presented some of her recently published work, "Multivalent Display of Functional Split Proteins on  $\beta$ -Sheet Self-Assembled Fibrils," (published in *Organic & Biomolecular Chemistry* 2017, 15, 5279–5283) and received a Young Investigator's Poster Competition Award for her presentation.

**JEN URBAN**, a member of both the Nilsson and Krauss groups (in collaboration with Handy Gelbard in the University of Rochester Medical Center), has spent the last year heroically forging ahead in her project, the

application of quantum dots for super high resolution imaging of cellular processes relevant to Alzheimer's disease. Her project has demanded that she single-handedly (almost) configure microscope instrumentation (serious problem solving here), adapt analysis software, synthesize peptides, and functionalize quantum dots! The project is exciting, but she's truly doing the work that would probably be done by three separate students in a normal collaborative effort. She's made outstanding progress and now stands at the cusp of the breakthroughs she's been working toward for several years. In addition to her great work in the lab, Jen has also been quite well travelled in the last year. She presented the results of her work at the Single Molecule Biophysics Meeting (Aspen Center for Physics) in Aspen, CO and she also attended an HHMI MicroED Workshop at the Janelia Research Campus in Ashburn, VA. The latter workshop was an intensive course designed to train scientists to implement state-of-the-art MicroED techniques at their home institutions. She also spent two weeks in Japan on vacation, her first time outside of North America. We anticipate that by this time next year, Jen will have



Jennifer Urban at Single Molecule Biophysics Meeting 63

defended her Ph.D. thesis and will be well on her way to productive employment. She's recently been fascinated with the science and art of distilling spirits, so perhaps (?) she'll apply her skills to a career in that industry.

**JADE WELCH** continues 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. Jade's foundational work in this area resulted in the funding of an NIH R01 grant from the National Heart, Lung, and Blood Institute this year! Jade also attended the American Peptide Symposium in Whistler, BC, Canada funded by an American Peptide Society Travel Grant and presented her work on the "Functional Delivery of siRNA by Disulfide-Constrained Amphipathic Peptides." She also received a Department of Chemistry Weissberger Memorial Fellowship this year. Based on her outstanding progress, we anticipate that Jade will defend her Ph.D. thesis during the summer of 2018.

Two new students joined the Nilsson group in the fall of 2017. **BRITTANY ABRAHAM** grew up in Spencerport, NY and earned her B.S. degree in chemistry from SUNY Geneseo. She enters our program as a University Sproull Fellow. She conducted undergraduate REU research in the Nilsson group during summer 2016 and we're thrilled to have her as a longer-term member of the group. She will study the self-assembly of low molecular weight amino acid derivatives in the design of novel supramolecular hydrogels for biomedical applications. **ELENA QUIGLEY** comes from Hilton, NY and completed BS studies in biochemistry at SUNY Fredonia. She is interested in NMR characterization techniques and will apply this interest to the use of solid-state NMR techniques to characterize the molecular structure of supramolecular hydrogel materials, a new research area for the Nilsson group. We're very excited to have these students in the group and look forward to the next years of productive collaboration.

Some of our group alumni have had significant milestones in 2017. **PAUL RUBEO (M.S. '16)** left the lab at the end of 2016 to return to his career in high school education. He was an outstanding student and we were sad to lose him. He's a gifted teacher and felt strongly pulled back to the profession. He's been very happy and we're thrilled for him! Paul was married to his fiancé, Mikella, in September of 2017. Many of our group members were able to attend the wedding. We



*Danielle, Jen and Jade at Paul and Mikella's Wedding*

congratulate Paul and Mikella and give them our best wishes for a happy and productive partnership!

**ANNADA RAJBHANDARY (PH.D. '16)**, who completed her Ph.D. in 2016, returned to her native Nepal to a research position at the Research Institute for Bioscience and Biotechnology. She recently received her first independent research grant (a UNESCO grant through the World Academy of Sciences Program) to continue aspects of her hydrogel work in the Nilsson group. We'll lend some collaborative work to assist her with some aspects of her project. We congratulate her on this success!

**JOHN DIMAIO (PH.D. '15)** completed his studies at the Law School at the University at Buffalo in the 2017. He has passed the bar exam and is currently working as an intellectual property attorney at Hodgson Russ in Buffalo, NY. We still see John frequently and he is thriving in his work, where he enjoys constant exposure to new and interesting science on a daily basis.

**TODD DORAN (PH.D. '11)**, who completed his Ph.D. work in 2011, completed his postdoctoral appointment with Professor Thomas Kodadek (Scripps Research Institute). He has moved to his first independent faculty position at the University of Minnesota in the Department of Medicinal Chemistry. Brad recently had the opportunity to host Todd's postdoctoral advisor, Tom Kodadek, as a seminar speaker in Rochester and Tom gave Todd glowing praise, indicating that Todd is among the very best postdoctoral researchers he has had the pleasure to work with. I'm confident Todd will find great success in his independent work. Todd and Brad have been working together for the last several years to edit a volume of the *Methods in Molecular Biology*



book series on Peptide Self-Assembly. We have delivered the final documents to the publisher and look forward to seeing the book in print!

The Nilsson group has continued to benefit from the energy of outstanding undergraduate research students. **JANSON HO**, a University of Rochester student in chemical engineering, spent the last several years conducting research in the Nilsson group, coauthored a recently submitted manuscript based on his work in our group. He is nearing completion of his degree in chemical engineering. **CHENGYENG LI (B.A. '17)**, another University of Rochester undergraduate, finished his chemistry degree in 2017 and is seeking acceptance into Pharmacy School. **PRESTON HOLLOPETER** and **MATT WATROUS** both contributed to our research efforts in the last year. Matt participated in the summer REU program and will continue his work on low molecular gelators this year. **CHEN CHEN** is conducting his senior thesis research in the Nilsson group in the area of peptide self-assembly. He will finish his degree this spring and is currently juggling many offers to top graduate schools in Chemical Biology for next year. He's been an outstanding student and we're confident he'll be a phenomenal graduate student as well. In addition to these talented students, **JASMINE GOMEZ (SUNY OSWEGO)** and **HYERIN YOON (UNIVERSITY OF ROCHESTER)** also conducted summer REU research in the Nilsson group during 2017. They made significant progress in their work in a short period of time and were

excellent additions to the group during their time at the University of Rochester.

In addition to managing our research efforts, Brad continued his work this year as chair of the Harrison Howe Award Committee (Rochester Section of the American Chemical Society), Chair of the Department of Chemistry Graduate Studies Committee, and teaching the first semester Organic Chemistry lab (CHM 207) and Bioorganic Chemistry and Chemical Biology (CHM 440). He is teaching Biological Chemistry (CHM 262/462) for the first time this Spring. Brad was also elected as Treasurer of the American Peptide Society during 2017, leaving him responsible for the management of the Society's endowment and finances. This is a new challenge he's still adapting to. At home, Brad and Trista's four kids are growing up quickly. Liam and Sadie are both at Brighton High School and Gavin is in his last year at French Road Elementary School. School, music, drama, and sports keep them and Mom and Dad busy. Their oldest daughter, Emma, has taken a gap after her first year of college at Brigham Young University to serve an 18-month LDS mission to Sweden. She's been in Sweden for almost two months and we love hearing about how great Sweden is and hearing about her struggles to learn Swedish when everyone speaks English! It's hard to believe that Gavin wasn't born yet and the other three were still so small when we first moved to Rochester. We're looking forward to another year of challenges and success in the lab, the classroom, and at home.



*The Nilsson Group (L to R): Jennifer Urban, Jade Welch, Danielle Raymond, Elena Quigley, Brittany Abraham, Bradley Nilsson*

# Lewis J. Rothberg

Professor of Chemistry

Ph.D. 1983, Harvard University



## RESEARCH INTERESTS

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

## CONTACT

rothberg@chem.rochester.edu

**LEWIS ROTHBERG'S** group research efforts have focused primarily on exploiting confocal microscopy of single conjugated polymer chains to understand morphological effects on their photophysics and on using delayed photoluminescence to understand charge recombination processes in electroluminescent organic materials. **RAJ CHAKABORTY** graduated with his doctorate in Materials Science in early 2017 and took employment at a local startup that develops materials for organic light-emitting diodes (OLEDs), Molecular Glasses. A new Ph.D. student **LIWEI WANG** got off to a fast start and has mastered confocal microscopy to spearhead our single polymer chain efforts. Their efforts have been supplemented by **XIN HUANG** (Materials Science MS) who is making excellent progress on reflective interferometric detection of antibodies, and a number of talented undergraduate students. **PAUL WRONA (B.S. '17)** completed a remarkable senior thesis doing Monte-Carlo modeling of single polymer chain photoluminescence using parallel computing methods on the University supercomputer and setting the stage for experimental and theoretical work he is now pursuing at Berkeley. **YONGLI LU** (Chemical Engineering undergraduate) has continued to amaze with new studies on how morphology affects delayed luminescence in conjugated polymers and has also completed work about to be published with collaborators Prof. Linda Peteanu (Carnegie Mellon) and Prof. Eric Fossum (Wright State) on novel materials exhibiting blue thermally activated delayed fluorescence that have potential for OLED technology. Yongli's insight also added considerably to some of Raj's thesis work and he coauthored a paper explaining magnetic field effects on delayed luminescence in conjugated polymer films. **TIANHAO YU** (Chemical Engineering undergraduate) has worked in the lab on a project characterizing new host materials for OLEDs with Molecular Glasses that was highlighted in the Rochester Review. Finally, **LEO ORSINI**, a talented first year student,

worked over the summer with us pioneering a new direction for the lab, studies of fluorescent conjugated polyelectrolytes. Colleagues **DR. RALPH YOUNG** and **DR. AL MARCHETTI** continue to work actively with the group and, more recently, we are also interacting with **DR. DAVID WEISS** from Molecular Glasses whose expertise in charge transport in organic materials has brought new insights and technology to the lab.

Lewis presented invited talks on the delayed luminescence research at the Spring ACS meeting in San Francisco and at the Optical Probes 2017 meeting in Quebec City during the summer. The OP2017 was the 13<sup>th</sup> in a thriving and still growing series that Lewis started with colleague **PROF. VALY VARDENY** at the University of Utah way back in 1994. Lewis remains on the organizing committee and has attended every single meeting in the series. Lewis attended a gratifying and memorable symposium held at the University of Utah in the Fall honoring **VALY VARDENY** on his 70<sup>th</sup> birthday ("Valyfest") where



Professor Valy Vardeny at Valyfest



many old friends in the conjugated polymer research community reunited. Lewis gave a talk there about **BEN MARTIN'S (PH.D '16)** single chain conjugated polymer luminescence work. There will be a companion Festschrift to be published this year.

Teaching was an even greater focus for Lewis than usual this past year. He taught the advanced spectroscopy lab (CHM 232) and, along with a ton of help from Deb Contestabile and student assistants, Dylan Gaeta (BA '16) and Prof. Katie Knowles, has updated John Muentner's excellent and legendary lab manual, the "Green Monster". Lewis also had the great privilege of teaching quantum chemistry (CHM251) for a second time and it was just as rewarding as the first. It's hard to imagine a more amazing intellectual trek and remains a thrill to engage with students grappling with the bizarre landscape of quantum theory. Finally, Lewis taught general chemistry (CHM 132) in the spring and substantially modified the course to focus on contemporary issues in environmental chemistry that reflect the thermodynamics and quantum mechanics in the syllabus. For example, enthalpy was discussed in the context of frontier research in energy production, electrochemistry in the context of hydrogen fuel cells, the periodic table in the context of elemental scarcity, spectroscopy in the context of Greenhouse gases and kinetics/catalysis in the context of ozone depletion and artificial photosynthesis. Lewis gave a talk about his experience with the new format and content at a "teach-in" for the University community in March. The course revision has stirred Lewis' passion around scientific literacy for the general public and he is taking sabbatical in 2018 to obtain training in scientific communication while working on case studies of chemistry in sustainability. He hopes to produce a book and companion materials focused on Chemistry for Citizens, as well as to continue to enrich the teaching of general chemistry to our own students. As a companion effort, Lewis is becoming more engaged in sustainability efforts on campus including participating on the Hutchison Hall building sustainability committee and in an effort to make a planned extension to Hutchison be a net zero energy addition. As part of the Center for Energy and Environment seminar series, Lewis hosted outstanding presentations by Patrick and J. Drake Hamilton last Spring. Patrick is Director of Global Change Initiatives at the Minnesota Museum of Science while J. Drake is science policy director for Fresh Energy, a non-profit that promotes the use of renewable energy.

The Materials Science program at the University, a Ph.D. and M.S. granting program of nearly 50 students, continues to thrive with **GINA EAGAN** helping to fill the

students' needs while driving further innovation. Lewis remains program director and has continued to push pedagogical initiatives such as pre-seminar meetings and soft skills training. This year we are continuing to enhance the conference series and web page as well as develop programs to seed more collaborative research and shared infrastructure amongst the materials faculty.

In addition to continuing research relationships with local organic electronics companies, Molecular Glasses and OLEDWorks, Lewis continues his consulting work for Chiral Technologies, the company that bought Diffinity Genomics which was spun out of the lab in 2005. Chiral has continued to sell the Diffinity product, Rapid Tip, making great strides this past year in manufacturing cost and consistency. Colleague Prof. Ben Miller's company, Adarza Biosystems, also based on technology from the lab, has had a very exciting few years and greatly expanded while establishing a headquarters in St. Louis. Lewis and Ben have both perennially given talks about entrepreneurship for the NSF summer research program students and shared their experiences with commercialization of University research.

The graduate fellowship fund for Chemistry students in honor of **ESTHER CONWELL** continues to grow. Lewis and Shelby are grateful to those who joined us in contributing. Shelby has taken new employment as Chief Technical officer of a small local startup aiming to commercialize novel electronic packaging technology, Mosaic Microsystems. Charles is a high school sophomore taking advanced history courses and doing model United Nations and made the junior varsity basketball team. Vivian became Bat Mitzvah in May and continues a busy schedule of acting, music, dance and cross-country running while excelling academically. Lewis enjoyed his 40<sup>th</sup>(!) reunion of the UR class of 1977 this year.



# 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 intermediate and high energies; non-equilibrium transport phenomena; thermodynamics of nuclear disintegration and transmutation; the equation of state of nuclear matter. Beyond the mean field: Nuclear particle correlations and cluster effects in nuclear astrophysics. Light-ion reactions in a thermonuclear environment. Transport of tritium in metals, including chemi- and physi-sorption.

## CONTACT

[schroeder@chem.rochester.edu](mailto:schroeder@chem.rochester.edu)

**W. UDO SCHRÖDER'S** Nuclear Science Research Group has continued research in radio-chemistry, specifically the dynamics of heavy- and light-ion induced reactions, and engages in advanced detector development. Laser Ion Acceleration for Nuclear Science (LIANS) has grown into an actual project pursued in collaboration with groups at the UR Laboratory for Laser Energetics (LLE). The radio-chemical experimental study of tritium transport in metals has yielded interesting and challenging results demanding further, specialized experimentation and analysis. Experience gathered in this field during the last five years turns out to be instrumental also in the development of the LIANS triton beam platform. In a parallel but related project, a first experiment has utilized the intense neutron flux ( $\sim 10^{14}$  per 'shot') produced at the LLE-Omega facility in each laser-induced inertial-confinement fusion event. Here, neutron-induced breakup of deuterium was detected and analyzed.

The most recent Ph.D. graduates from the Nuclear Science Research Group are all doing well: Former student **SHETH NYIBULE** teaches Freshman physics at the Rochester Institute of Technology, **ERIC HENRY** is busy developing the next generation of semiconductor computer chips at INTEL, while **MATT SHARPE**, just promoted to a research associate position at LLE, will continue working on the tritium fuel cycle and remain a resource for our development of a tritium beam for the LIANS platform at the Omega/EP facility.

Meanwhile a new generation of nuclear graduate students has taken on the scientific challenges left on their desks. Graduate students **ARNOLD SCHWEMMLEIN** and **CODY FAGAN** have received their respective M.S. degrees in physics or chemistry. Arnold has been working on GEANT simulations of experiments on laser-induced light-ion reactions, with  $^9\text{Be}(d,n)^{10}\text{B}$  as

a first test case. His main task is to design and test an adaptation of the LIANS platform for unique triton beams. To supplement his training in applied nuclear reaction physics, Arnold attended a 10-day TRIUMF summer school on astrophysics at Vancouver/Canada.

On the radio-chemical side, Cody has embarked on a detailed study of surface effects in tritium transport, absorption, storage, and desorption by metals. He has acquired specialized skills and can now enjoy using a host of advanced equipment and methods (ALD for

## Nuclear Particle Correlations and Cluster Physics

Wolf-Udo Schröder, *Editor*



 World Scientific

Wolf-Udo Schröder new book cover



modification, XPS, SEM, AFM for analysis) available on Campus for the study of metallic surfaces. The photograph shows him at his plasma desorption setup, now at LLE. As the most recent addition to the group, graduate student **DANIEL BASSLER** has finished his teaching assignments in Chemistry. With Cody, Dan is now busy testing various methods to alter metal surfaces in a controlled fashion.

Results of the group's research have been reported in journal and book publications, as well as in invited lectures. Udo has published another book (WSPC), see picture of cover. This most recent book reports on Nuclear Particle Correlations and Cluster Physics and represents joined efforts by more than 20 research teams on four continents. In September, Udo presented an invited lecture at the International Workshop on Finite

System in Nonequilibrium in Natal/Brazil. During a week in summer at the ACS Summer School on Nuclear Chemistry at Brookhaven National Laboratory, he also gave a course on nuclear structure concepts and applications.



*Cody at plasma setup*

## Douglas H. Turner

Professor of Chemistry

Ph.D. 1972, Columbia University



### 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.

### CONTACT

turner@chem.rochester.edu

Like nuclei in an NMR spectrometer, Doug Turner is undergoing a transition. He is in slow exchange between being an experimentalist and a computational chemist. Doug has been cleaning out the group's -80 °C freezer and soon will be the only biohazard in the lab. Fortunately, **DAVE MATHEWS (PH.D. '01, M.D. '03)** and the Mathews group are giving Doug continuous stimulation for his transition. For several years, the groups have had monthly or more often meetings of one kind or another. An extended set of such meetings with graduate students, **LOUIS SMITH** (Biophysics) and **JIANBO ZHAO** (Chemistry) produced a long review of the current state of using physical principles to predict RNA energetics and 3D structure.

Predictions for RNA are often poor, so there is a lot left to discover. **ANDY KAUFFMANN** in collaboration with **SCOTT KENNEDY** and **JIANBO ZHAO** provided an example of this by publishing an NMR structure of a duplex with a symmetric internal loop containing six

GA and two AC pairs. Only one (MC-sym) of three commonly used prediction programs successfully predicted the hydrogen bonding in the GA pairs, even though they form two "3RRs" motifs commonly found in other RNAs as originally identified by Scott.

Sometimes, it is even difficult to predict secondary structure when GU pairs close a loop. **KYLE BERGER** has discovered this is even true for RNAs as short as 10 nucleotides. His work has been submitted for publication in collaboration with the Mathews group, Scott Kennedy, **BRENT ZNOSKO (PH.D. '04)**, and **SUSAN SCHROEDER (PH.D. '02)**.

Doug has been interested in stacking interactions since his graduate work on the kinetics of proflavin stacking and his initial Rochester research with **GREG DEWEY (PH.D. '79)** on the kinetics of polyadenylic acid stacking. In the last several years, NMR experiments and computations published with Scott Kennedy, **ILYAS**

**YILDIRIM (PHYSICS PH.D. '08), JASON TUBBS (PH.D. '13), and DAVE CONDON (PH.D. '15)** provided comparisons between spectra for unpaired tetramers and predictions from molecular dynamics simulations. Again, the comparisons revealed that much is left to discover. The group's papers have been frequently cited and noticed by computational groups, which led to a collaboration between Jianbo and Doug with the Bussi group in Trieste, Italy.

It has been fun to follow the careers of former members of the group. **MATT DISNEY (PH.D. '02)** won the 2016 Tetrahedron Young Investigator Award in Bioorganic and Medicinal Chemistry. He was featured in a November 2017 C&E News article titled, "The RNA drug hunters." Matt's name started the article with the M four columns high and 15 spaces long, so Doug now calls him Big M (assuming that has not already been assigned to a rapper). Matt has also started a company, Expansion Therapeutics, for drug discovery. Another professor/entrepreneur, **JOHN SANTALUCIA, JR. (PH.D. '91)**, won a Michigan "2016/2017 Fast Track" Award because his company, DNA Software Inc., had revenue growth of over 20% for three years in a row. His company excels at measuring thermodynamics and predicting nucleic acid sequences for defined purposes. **JIM HART (PH.D. '08, M.D. '10)** was promoted to Associate Medical Director at Abbott Labs in Dallas. Fortunately for Abbot Labs, two Turner alumni Jim hired, **TIANBING XIA (PH.D. '99)** and **TIAN JIANG (PH.D. '15)**, remain in Jim's former unit. **SUSAN SCHROEDER (PH.D. '02)** won a Burroughs Wellcome Collaborative Travel Grant to partially support a year sabbatical in the lab of **PHIL BEVILACQUA (PH.D. '93)**. They collaborate on studies of RNA in plants. Interestingly, Susan and Phil are faculty at the University



*Doug in the lab*

of Oklahoma and Penn State, respectively, which both had football teams ranked in the top 5 at some point this year. In an attempt to join that ranking, Ilyas's Florida Atlantic University finished 11-3 this year and won the Cheribundi Tart Cherry Boca Raton Bowl under new coach, Lane Kiffin. Coach Kiffin then signed a 10 year contract with a base salary of roughly  $\$1 \times 10^6$  per year. Strangely, none of the Turner alumni mentioned football this year. Maybe they should ask the football coaches for advice for the Chemistry Departments.

Doug enjoyed giving a talk at the Telluride RNA Dynamics Meeting in July and listening to talks by Dave Mathews and Ilyas Yildirim. He also enjoyed visiting his Ph.D. advisor, Norman Sutin and wife Bonita. Norman is an amateur magician and it is magic just to talk with him. Doug also attended his 50th college reunion, which was a magical time machine since none of his four roommates have changed. It was also magical that after 50 years, Doug was made an honorary member of Phi Beta Kappa. It only took his son, Ricky, 4 years.



*The Turner Group (L to R): Jianbo Zhao, Kyle Berger, Professor Doug Turner, Andrew Kauffmann, Scott Kennedy*



# Daniel J. Weix

Associate Professor of Chemistry

Ph.D. 2005, University of California, Berkeley



## RESEARCH INTERESTS

Transition-metal catalyzed reactions; synthetic organic chemistry; methods development; study of reaction mechanisms; reductive chemistry; stereoselective transformations.

## CONTACT

weix@chem.rochester.edu

Research in **PROFESSOR DANIEL WEIX'S** group is focused on the development of new, catalytic methods for forming C-C and C-X bonds, with a particular emphasis on understanding mechanism and the use of first-row transition metals. The major focus of the group continues to be the selective cross-coupling of two electrophiles and the use of earth-abundant, first-row metals. Big advances this year were in the advent of semiconductor quantum dot photoredox catalysis (collaboration with Todd Krauss), expansion of the scope of cross-electrophile coupling partners to include Csp carbons, primary alkyl halides, and heteroaryl halides, and a convenient trick for removing triphenylphosphine oxide. To commemorate the growth of cross-electrophile coupling over the past decade, Dan co-organized an ACS Symposium at the Fall meeting. Finally, this update is also a fond farewell because Dan moved to the University of Wisconsin in July of 2017.

Dan continued teaching freshman organic and honors organic lab in 2016, a wonderful teaching assignment that has allowed him to meet so many great students. In addition to the wonderful work of the undergraduate and graduate teaching assistants in these courses, Dan and his students benefitted from the newest instructional faculty member, **JOHN-CARL OLSEN**. JC brought

demonstrations to a new level in 171, adding in demos for nearly every unit, and helped out with lecturing in 210 with great success. It was wonderful leaving on such a high note, but Dan will miss the students and staff that made teaching such a joy at Rochester!

The group was fortunate to be recognized with a variety of awards and honors this past year. On top of the departmental chemistry junior award, **NORMAN ZHAO (B.S., '17)** was awarded an NSF Graduate Research Fellowship Award! This makes for a total of six NSF Graduate Fellows from the Weix group at Rochester (2 undergraduate and four graduate)! **AMANDA SPIEWAK** was awarded a W. D. Walters teaching award, joining a long tradition of Weix group members to win this great honor. To support travel to the ACS Green Chemistry and Engineering Meeting in June, **MATTHEW GOLDFOGEL** was awarded a travel grant from the ACS Green Chemistry Pharmaceutical Roundtable in June. Even more exciting, Matt was awarded a prestigious NIH postdoctoral fellowship in August. Finally, Dan was elected a fellow of the American Association for the Advancement of Science (AAAS) and won a travel award from the Japan Society for the Promotion of Science (JSPS). Being elected an AAAS fellow is a great honor and Dan is humbled to be among the many Rochester faculty fellows. The JSPS award funded Dan's trip to Japan in May, where he visited ten institutions during a two-week trip, renewing many old friendships and making many new ones. These awards are a reflection of the intelligence and creativity of the group members, past and present.

This year included many changes both related and unrelated to the move. Emily Johnston worked with Astrid Olivares during her year at Rochester. Emily joined us from University of Bristol and took full advantage of what Rochester had to offer. **NORMAN ZHAO** graduated in May and moved to the University of



*The Weix Group at the airport*

Chicago for graduate studies in Chemistry. At the same time, **SEOYOUNG KIM**, **TARAH DIBENEDETTO**, and **AMANDA SPIEWAK** all were awarded Masters degrees. **KIERRA M. M. HUIHUI (PH.D. '17)** defended her PhD in June and moved to a new job in Oregon at Impria. **TARAH A. DIBENEDETTO** passed her oral exam in July. **AMANDA SPIEWAK** passed her oral exam in Wisconsin in December and Seoyoung will finish hers in January. **ASTRID M. OLIVARES** completed her third-year talk on single-electron-transfer steps in water oxidation catalysis. Astrid and Tarah both decided to stay in Rochester and moved to join Prof. William Jones's group in November after an excellent tenure in the Weix group. **ALEX CALLAHAN** (class of 2018) worked in the LLE this summer showing off his synthetic chops and started work in the Bren lab this Fall for his senior thesis. The group also welcomed the last Rochester class, **KEVIN GARCIA** and **DANIEL ENNY**, as well as our first Wisconsin class, **VICTORIA LONGLEY**, **BRETT SCHNEIDER**, and **MICHELLE AKANA**. Kevin graduated from Bucknell, where he worked with Robert Stockland. Daniel is a Lehigh graduate. While there he conducted research with Robert Flowers III. Victoria graduated from the University of Minnesota where she worked with Wayne Gladfelter. Brett graduated from St. Mary's University. During his undergraduate days, Brett worked in a number of labs at St. Mary's (Larionov), UTSWMC (Bauta), and UTSA (MacMillan). Michelle also graduated from St. Mary's University. Michelle, too, worked in a number of labs at St. Mary's (Galaldeen, Schoonover), UT Health Science Center (Ivanov), and UTSA (Zhao). Finally, new postdocs **MATTHEW GOLDFOGEL** (PhD '16 from UNC Chapel Hill) and **JIANG WANG** (PhD '17 from University of Arkansas) joined in September. Matt is a late-metal and hydrofunctionalization specialist from the Meek lab and Jiang is a specialist in photoredox chemistry from the Zheng lab. Current postdoc **LIANGBIN HUANG** and wife Ji welcomed their first child, Mochuan (English name of Lucas), in May. The family moved to Madison in August and is adjusting to life in the Midwest.

The move to Wisconsin means that Stella and Dan's children, Elliott (12), Madeleine (10), and Amalia (8), will have the opportunity to get to know their extended family much better in the coming years, but we will all miss Rochester terribly. Rochester has been a wonderful home for the family for the past nine years and we leave you with a short, incomplete list of the places/events we will miss most: Stony Brook State Park, the Seneca 7 race, Jeremiah's Tavern, Dinosaur BBQ,

Lento's Tuesday happy hour, Adventurerock Climbing Gym, Rochester Parkour, Sultan, Wegmans, and Le Petit Poutine. Rochester will always be 'home' to us!

In group alumni news, **SOUMIK BISWAS** (postdoc) had a year of big events – Moumita and he welcomed their first son, Aman, in February and soon the growing family will move to San Diego so that Soumik can start his new job at WuXi AppTech. There were also a lot of new jobs among alumni: **LUKIANA AMEDZO (PH.D. '15)** started a new job at PTC Therapeutics. **YANG ZHAO (PH.D. '15)** took a job as the Chief Technology Officer at Francool Technology (Shenzhen) Corporation, Ltd. Finally, we had two alumni with big news in the medical field. First, **ADAM LEE (B.A. '12)** completed his MBBS degree (Bachelor of Medicine Bachelor of Surgery), getting Honors in Internal Medicine. Second, **MATTHEW LOVELL (B.S. '14)** started medical school at Wright State Boonshoft School of Medicine in Dayton, Ohio. Congrats to everyone!

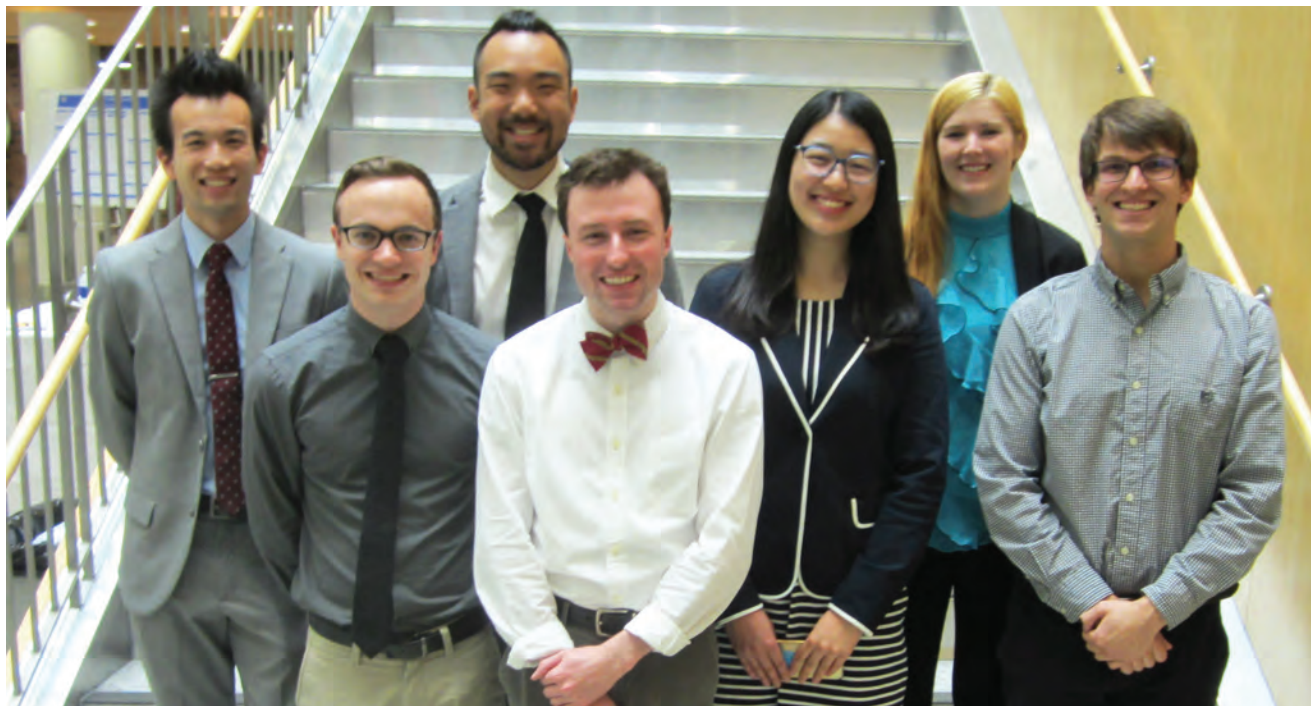
A final note: Dan is grateful to the faculty, staff, and administration at the University of Rochester for giving him a once-in-a-lifetime chance to get paid to research things he is interested in and teach amazing students! Meliora!



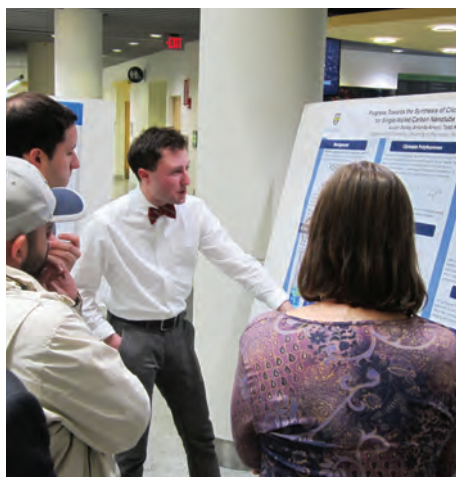
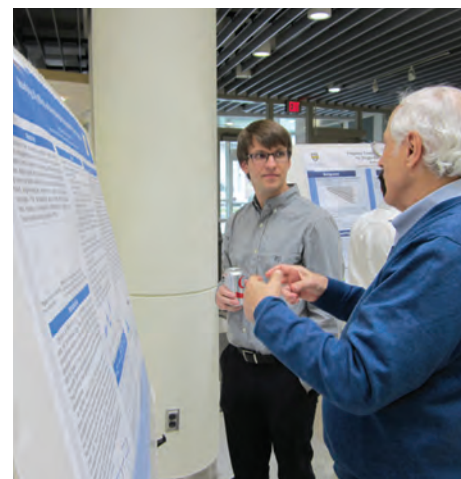
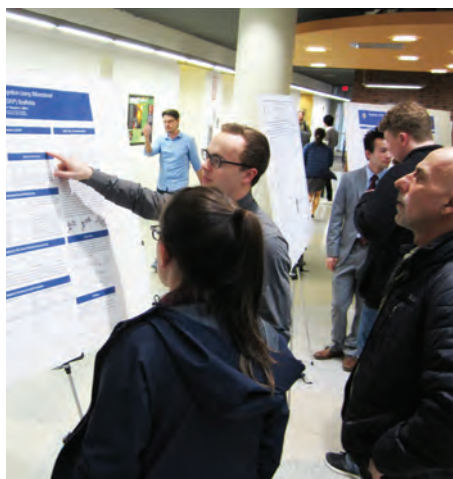
The Weix Group



# Senior Poster Session



Class of 2017 Senior Thesis Poster Session  
1st row: Norman Zhao, Hayden Carder, Austin Bailey, Yifei Liang, Paul Wrona.  
2nd row: Cory Chen, Jessica Freeze.





# Commencement

## Bachelors and Masters Degrees Awarded in Chemistry

### 2017 BACHELOR OF SCIENCE

Austin Bailey \*  
Cory Chan  
Jessica Freeze  
Yifei Liang†

Fulei Peng \*\*  
Paul Wrona  
Norman Zhao

### 2017 BACHELOR OF ARTS

Jehong (Daniel) Ahn  
Gyeong Bang  
Lauren Bolz†  
Rachel Bonn  
Lujain Felemban  
Ping He\*\*  
Charlotte Humes \*\*  
James Kostka

Chengyang Li  
Shiyang (Stanley) Li  
Joshua McGough  
John Passanisi  
Gavin Piester†  
Aiyana Smith  
Zihan Zhang

<sup>1</sup>Distinction   <sup>2</sup>High Distinction   <sup>3</sup>Highest Distinction   †Phi Beta Kappa  
\*Take 5 Scholar (beginning)   \*\*Take 5 Scholar/KEY Program (finishing)



*Class of 2017 Bachelor's Degree Recipients*

### 2017 MASTER OF SCIENCE

Somjit Bhar  
Sutirtha Chowdhury  
Tarah DiBenedetto  
Cody Fagan  
Antonio Garzon Ramirez

Seoyoung Kim  
Jennifer Le  
Xinyang Li  
Rachel Meyer  
Eric Moore

Justin Niziol  
Brittney Petel  
Jeffrey Sears  
Amanda Spiewak  
Mehrinn Tariq

Antonio Tinoco Valencia  
Lauren VanGelder







# Doctoral Degrees Awarded in Chemistry

*Ph.D. Degrees Conferred on March 17, 2017*

## Jill Caputo

*I. Nickel-Catalyzed Additions to Imines and Aldehydes and II. Photoredox Catalysis with Quantum Dot Catalysts in Carbon-Carbon Bond Forming Reactions*

Advisor: Daniel Weix

## Stephanie Daifuku

*Insight into Iron C-C Cross-Coupling Catalysis through Structure, Bonding and Mechanism*

Advisor: Michael L. Neidig

## Adam Feinberg

*I. Fragmentation Mechanisms of Aryltrialkylsilane and –Germane Cation Radicals II. Alkoxy Radicals as Hydrogen Atom Donors*

Advisor: Joseph Dinnocenzo

*Ph.D. Degrees Conferred on August 31, 2017*

## Douglas Tusch

*Part I. Studies Towards the Total Synthesis of (-)-Apoptolidin A Part II. Hydroxymethylation of Aldehydes and Its Application to (-)-Rasfonin*

Advisor: Robert K. Boeckman, Jr.

## Lifeng Xiao

*I: Studies Toward the Total Synthesis of (-)-Apoptolidin A; II: Bone Targeted Bis-phosphonate Conjugates with Releasable Payloads as Prodrugs for the Treatment of Bone Metabolic Diseases*

Advisor: Robert K. Boeckman, Jr.

## Kierra Huihui

*Nickel-Catalyzed Coupling of N-Hydroxyphthalimide Esters with Aryl Iodides and Reductive Conjugate Addition Reactions with Enones*

Advisor: Daniel Weix

*Ph.D. Degrees Conferred on October 13, 2017*

## Jared Kneebone

*Electronic Structure and Reactivity in Iron-Catalyzed Carbon-Carbon Cross-Coupling Reactions*

Advisor: Michael L. Neidig

## Miles Wilklow-Marnell

*Manipulation of Carbon-Element Bonds by Pincer Ligated Iridium Complexes*

Advisor: William D. Jones



*The Martin Brewer Anderson statue (J. Adam Fenster)*



# Student Awards

## DEPARTMENT AWARDS

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

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.



2017: Lauren Bolz

### John McCreary Memorial Prize

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. John's career maintained its exemplary character until his untimely death in 1983. The award, given to an outstanding senior undergraduate student, consists of a cash prize.



2017: Gavin Piester

### ACS Rochester Section Award

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.



2017: Paul Wrona

### ACS Inorganic Chemistry Award

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



2017: Norman Zhao

### ACS Organic Chemistry Award

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



2017: Yifei Liang

## ACS Physical Chemistry Award

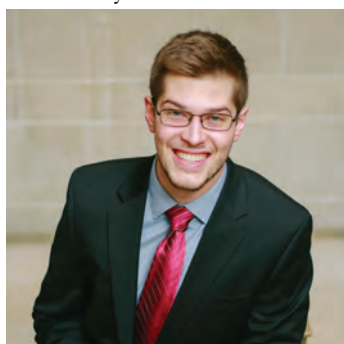
This award is intended to encourage student interest in physical chemistry and to recognize students who display an aptitude for a career in the field. The award consists of a personalized certificate and souvenir item from ACS, as well as a cash prize and certificate from the department.



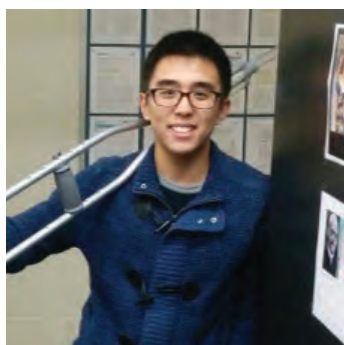
2017: Austin Bailey

## Chemistry Department Award

The Chemistry Department Award is given to seniors in recognition of outstanding scholarship in the study of chemistry.



2017: Joshua McGough



2017: Fulei Peng

## COLLEGE AWARDS

### Janet Howell Clark Prize

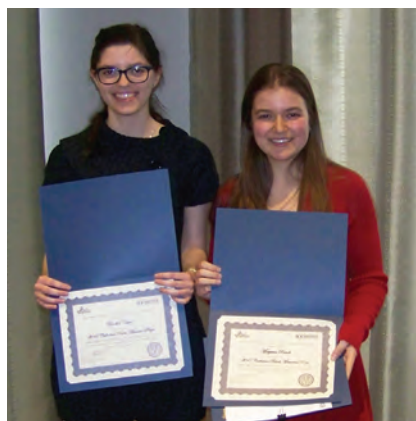
The Janet Howell Clark Prize is awarded annually to the senior woman who has shown the greatest promise in creative work in either astronomy, biology, chemistry, or physics, and who has shown outstanding versatility in the mastery of allied fields. Selection is based on recommendations by the respective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



2017: Yifei Liang

### Catherine Block Memorial Fund Prize

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.



2017: Rachel Clune, Merjema Purak



## Irene Bush Steinbock Award

The award was established by Irene Bush Steinbock “in memory of the late Dean Annette Gardner Munro, whose kindness and graciousness was a great inspiration to me during my years of study at the University of Rochester.” This award is given to a senior in the School of Arts and Sciences who has made the most noteworthy contribution to human relations. Selection is based on recommendations which are evaluated by a committee appointed by the Dean of the College. The award consists of a cash prize and recognition at a special senior ceremony the Saturday of Commencement.



2017: Lauren Bolz



2017: Gavin Piester

## TEACHING AWARDS

### Carl A. Whiteman, Jr. Teaching Award

This 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.



2017: Austin Bailey, Lauren Bolz, Jessica Freeze, James Kostka, Paul Wrona

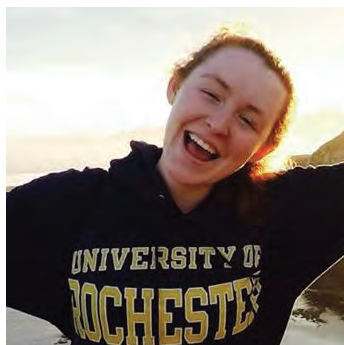
## Junior Scholar Award for Juniors

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



2017: Yongli Lu, Rachel Clune, Chen Chen, Hayden Carder, Alex Callahan, Merjema Purak, Alyssa Flaschner

## PHI BETA KAPPA



2017: Lauren Bolz



2017: Yifei Liang

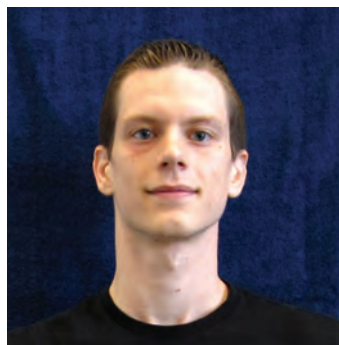


2017: Gavin Piester

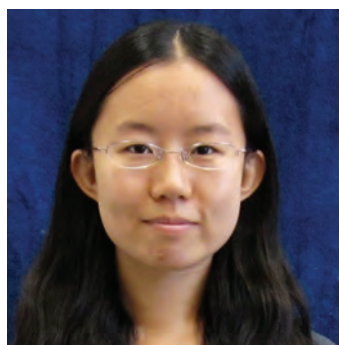
## ENDOWED DEPARTMENT FELLOWSHIPS

### Robert & Marian Flaherty DeRight Fellowship

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.



2017: Dylan Parsons



2017: Jianbo Zhao



## Moses Passer Fellowship

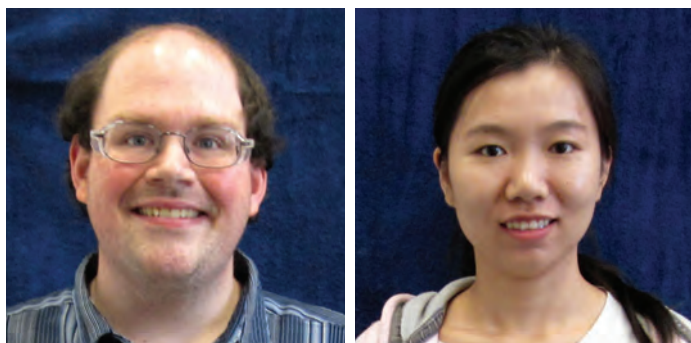
This endowed fellowship fund was established by Mrs. Dorothy Rosenberg-Passer in 2009 in memory of her husband, Dr. Moses Passer, who received his bachelor of science degree in chemistry from the University of Rochester in 1945 and his doctorate in organic chemistry from Cornell in 1948. After a distinguished 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.



2017: Jennifer Le

## Elon Huntington Hooker Fellowship

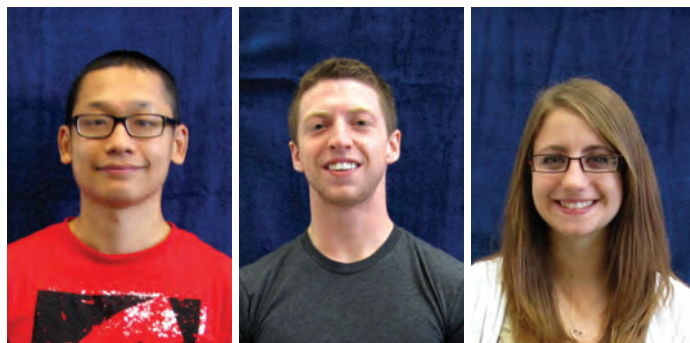
The Elon Huntington Hooker Fellowships are awarded from a gift from Mrs. Elon Huntington Hooker in memory of her husband, Elon H. Hooker, a graduate and, for many years, a trustee of the University. These fellowships are awarded in various fields of science, especially chemistry.



2017: Hanan Alwaseem, Stephanie Carpenter, Valerie Fleischauer, Kyle Rugg, Jing Yuwen

## Arnold Weissberger Fellowship

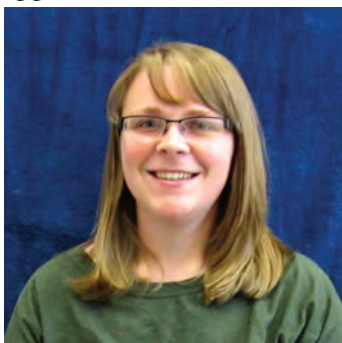
The purpose of the Weissberger Fellowship in Chemistry is to reward and encourage outstanding promise for productive scientific careers by advanced Ph.D. students. Each Fellow receives a substantial supplement for basic support and funds to travel to a major scientific meeting to report the results of his or her 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.



2017: Georgios Alachouzos, Sutirtha Chowdhury, Rebeckah Burke, Yixing Guo, Andrew Owens, Jade Welch

### **Samuel A. & Ellen F. Lattimore Fellowship**

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.



**2017:** Abigail Freyer



**2017:** Theresa Iannuzzi



**2017:** Brittney Petel



**2017:** Viktoria Steck

### **Robert L. and Mary L. Sproull Fellowship**

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.



**2016-2019:** Jesse Stroka

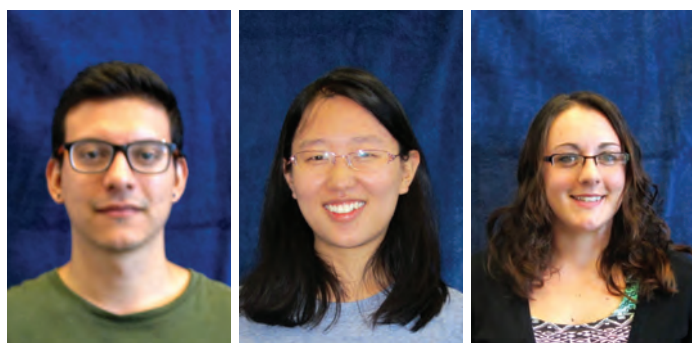
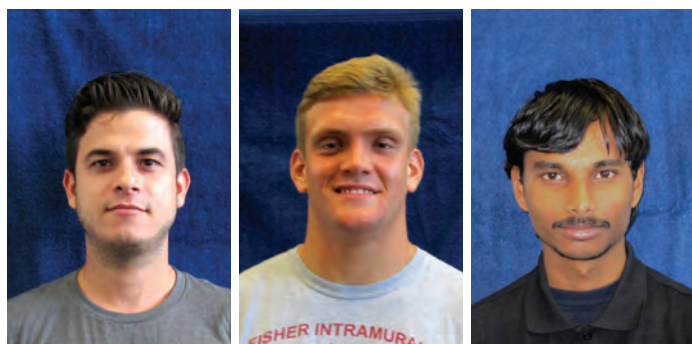
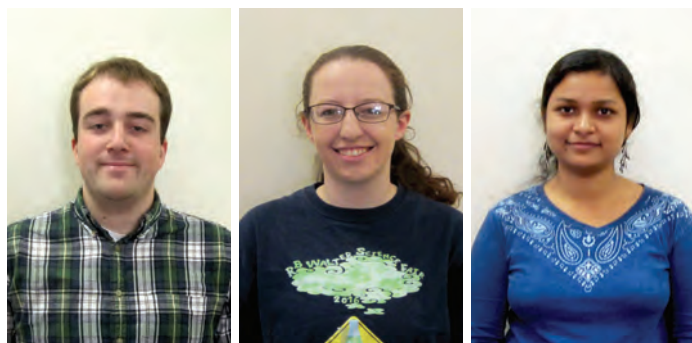


**2017-2020:** Brittany Abraham



## Sherman-Clarke Fellowship

The Sherman-Clarke Fellowship is a merit fellowship awarded to graduate levels students based on coursework and Teaching Assistant performance.



**2017:** Andrew Bortz, Emily Edwards, Maitrayee Ghosh, Connor Holt, Jacob Iannuzzelli, Trevor Tumiel, Jose Alvarez-Hernandez, Jordan Andrews, Arkajit Mandal, Leopoldo Mejia Restrepo, Liwei Wang, Nikki Wolford

## GRADUATE AWARDS

### W.D. Walters Teaching Award

This award recognizes outstanding undergraduate teaching by graduate teaching assistants. This award memorializes 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.



**2017:** Jordan Andrews, Shukree Abdul-Rashad, Antonio Tinoco, Nikki Wolford, Dylan Parsons, Sutirtha Chowdhury

### Outstanding Graduate Student Award

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.



**2017:** Abigail Freyer



*Hanan Alwaseem*

## ACS WOMEN CHEMISTS COMMITTEE/ ELI LILLY TRAVEL AWARD

**Hanan Alwaseem** was awarded the ACS Women Chemists Committee/Eli Lilly Travel Award, an award bestowed to women in science on the basis of their research accomplishments and merits. Hanan used the funds to attend the 254th American Chemical Society National Meeting in Washington D.C and present her latest results on developing chemoenzymatic routes for the functionalization and optimization of an antileukemic natural product. Hanan received the recognition at a public reception followed by a private dinner with the other awardees and the directorate of WCC and the ACS. Hanan was born in Yemen and grew up in Belvidere, Illinois. After obtaining her B.S. degree in chemistry from the University at Michigan-Dearborn, she joined our department and the Fasan research group. Her research focuses on the development and application of P450 catalysts for late-stage functionalization of complex natural products.



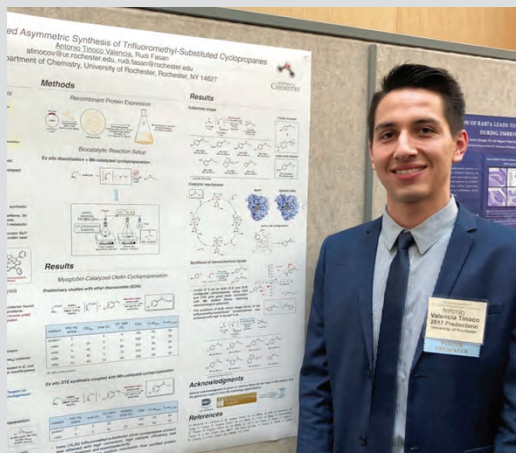
*Lauren Van Gelder in glove box*

## NSF GRADUATE FELLOWSHIP AWARD AND ELLIOT AND LAURA RICHMAN TRAVEL AWARD

**Lauren VanGelder** is a Rochester native who grew up in Brockport, NY. Lauren obtained undergraduate degrees in both chemistry (B.Sc.) and biomedical sciences (B.Sc.) at The University at Buffalo, SUNY, after which she returned to Rochester to pursue a Ph.D. in Chemistry in the Matson Group at U of R. She will be using the funds provided by the Elliot and Laura Richman Travel Award to travel to the Gordon Inorganic Conference in Maine in Spring 2018 to present her recent work on developing energy dense electrolytes for redox-flow batteries.

Lauren was the recipient of a prestigious NSF Graduate Fellowship Award in March 2017. She was also selected as the first prize winner in a poster contest at the “New York Battery and Energy Storage Technology Consortium (NY-BEST) Energy Storage Conference” held in October 2017 for her work on Vanadium-oxide Clusters as electrolytes for Redox Flow Batteries.



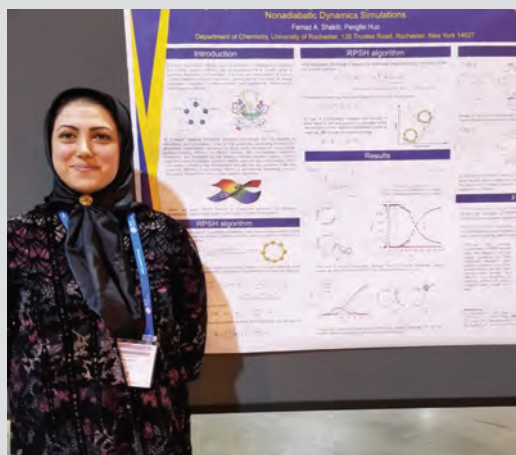


*Antonio at the 2017 Ford Fellows Conference, Washington, D.C.*

## FORD FOUNDATION FELLOWSHIP

**Antonio Tinoco Valencia** was awarded one of the prestigious Ford Foundation Fellowships, which are bestowed by the National Academies of Sciences, Engineering, and Medicine to predoctoral scholars in recognition of their promise for superior academic and scientific achievements. As a Ford fellow, Antonio attends a yearly meeting with other high-achieving scholars committed to diversifying the professoriate and using diversity as a resource for enriching the education of all students. Antonio was born

in Guanajuato, Mexico, and was raised in Los Angeles, California. He obtained his B.S. in Chemistry from California State University and joined the Department of Chemistry at the University of Rochester in 2015. Antonio is a member of Prof. Fasan's group and his research focuses on developing and investigating the mechanism of myoglobin-catalyzed carbene transfer reactions.



*Farnaz at the 2018 ACS computational chemistry award poster session, New Orleans, LA.*

## ACS WILEY COMPUTERS IN CHEMISTRY OUTSTANDING POSTDOC AWARD

**Dr. Farnaz A. Shakib** was one of the two awardees of the 2018 ACS Wiley Computers in Chemistry Outstanding Postdoc Award. This award is designed to assist postdocs in gaining visibility within the COMP community and in their transition to subsequent employment. Farnaz received this award and the recognition at a public reception in the 255th American Chemical Society National Meeting in New Orleans, presenting her work with Prof. Pengfei Huo on incorporating nuclear quantum effects into nonadiabatic

molecular dynamics simulation via ring polymer surface hopping. Farnaz obtained her B.S. degree in applied chemistry in Tabriz University, Iran, followed by a M.S. degree in Organic Chemistry. Switching to theoretical and computational chemistry, she joined Dr. Gabriel Hanna's group in the University of Alberta, Canada, where she received her Ph.D. in 2016. She joined the Huo group at the University of Rochester in 2016 as a postdoctoral scholar. Engaging in the continuous effort in Huo group to push the boundaries of quantum dynamics simulation techniques, her main focus at Rochester was on developing efficient and accurate methods to study the nonadiabatic dynamics of photoinduced proton-coupled electron transfer reactions in natural and artificial photosynthesis.

# Faculty Publications

## January 2017 - December 2017

### ROBERT K. BOECKMAN, JR.

Bone-Targeted Pharmacological Inhibition of Notch Signaling Decreases Resorption and Induces Bone Gain in Skeletally Mature Mice. J. Delgado-Calle; M. E. Olson; J. H. Nelson; E. G. Atkinson; K. McAndrews; L. F. Xiao; F. H. Ebetino; R. K. Boeckman; G. D. Roodman; T. Bellido, *J Bone Miner Res*, **2017**, *32*, S9.

A Novel Strategy to Target Chloroquine to Bone to Increase Its Anti-Resorptive Activity and Reduce Side-Effects. B. F. Boyce; Z. Yao; L. Xing; A. Ayoub; R. K. Boeckman; F. H. Ebetino, *Osteoporosis Int*, **2017**, *28*, S494.

### KARA L. BREN

Covalent bonding of heme to protein prevents heme capture by nontypeable Haemophilus influenzae. V. Sgheiza; B. Novick; S. Stanton; J. Pierce; B. Kalmeta; M. F. Holmquist; K. Grimaldi; K. L. Bren; L. V. Michel, *Febs Open Bio*, **2017**, *7*, 1778.

Engineered Biomolecular Catalysts. K. L. Bren, *J Am Chem Soc*, **2017**, *139*, 14331.

Locked and loaded for apoptosis. K. L. Bren; E. L. Raven, *Science*, **2017**, *356*, 1236.

Photoinduced charge separation in single-walled carbon nanotube/protein integrated systems. L. Kubie; A. R. Amori; S. Chakraborty; K. L. Bren; T. D. Krauss, *Nanoscale Horiz*, **2017**, *2*, 163.

Testing c-Type Heme Sources for Nontypeable Haemophilus influenzae. S. Stanton; J. Pierce; V. Sgheiza; K. L. Bren; L. Michel, *Faseb J*, **2017**, *31*.

Efficient and Flexible Preparation of Biosynthetic Microperoxidases. E. C. Kleingardner; W. B. Asher; K. L. Bren, *Biochemistry-US*, **2017**, *56*, 143.

### JOSEPH P. DINNOCENZO

Stereochemistry of Nucleophilic Substitutions on Benzyl-Stereochemistry of Nucleophilic Substitutions on Benzylsilane and-germane Cation Radicals: Application of the Endocyclic Restriction Test. M. S. Lenczewski; H. J. P. de Lijser; D. M. Turner; J. P. Dinnocenzo, *J Org Chem*, **2017**, *82*, 12112.

Aryltrimethylstannane Cation Radical Fragmentation Selectivities That Depend on Codonor: Evidence for Reactions from Heterodimer Cation Radicals. P. Luo; J. P. Dinnocenzo, *J Org Chem*, **2017**, *82*, 11052.

Cationic (Charge Shift) Exciplexes. J. P. Dinnocenzo; P. B. Merkel; S. Farid, *J Phys Chem A*, **2017**, *121*, 7903.

Multiple Intermolecular Exciplexes in Highly Polar Solvents. J. P. Dinnocenzo; A. M. Feinberg; S. Farid, *J Phys Chem A*, **2017**, *121*, 3662.

### RICHARD EISENBERG

Photochemical C-H Activation: An Early Story. R. Eisenberg, *Isr J Chem*, **2017**, *57*, 932.

Semiconductor quantum dot-sensitized rainbow photocathode for effective photoelectrochemical hydrogen generation. H. J. Lv; C. C. Wang; G. C. Li; R. Burke; T. D. Krauss; Y. L. Gao; R. Eisenberg, *P Natl Acad Sci USA*, **2017**, *114*, 11297.

### SAMIR FARID

Cationic (Charge Shift) Exciplexes. J. P. Dinnocenzo; P. B. Merkel; S. Farid, *J Phys Chem A*, **2017**, *121*, 7903.

Multiple Intermolecular Exciplexes in Highly Polar Solvents. J. P. Dinnocenzo; A. M. Feinberg; S. Farid, *J Phys Chem A*, **2017**, *121*, 3662.

### RUDI FASAN

Enzyme stabilization via computationally guided protein stapling. E. J. Moore; D. Zorine; W. A. Hansen; S. D. Khare; R. Fasan, *P Natl Acad Sci USA*, **2017**, *114*, 12472.

Stereoselective Olefin Cyclopropanation under Aerobic Conditions with an Artificial Enzyme Incorporating an Iron-Chlorin e6 Cofactor. G. Sreenilayam; E. J. Moore; V. Steck; R. Fasan, *Acc Catal*, **2017**, *7*, 7629.

Exploiting and engineering hemoproteins for abiological carbene and nitrene transfer reactions. O. F. Brandenburg; R. Fasan; F. H. Arnold, *Curr Opin Biotech*, **2017**, *47*, 102.



Design and Evolution of a Macrocyclic Peptide Inhibitor of the Sonic Hedgehog/Patched Interaction. A. E. Owens; I. de Paola; W. A. Hansen; Y. W. Liu; S. D. Khare; R. Fasan, *J Am Chem Soc*, **2017**, *139*, 12559.

New functional twists for P450s. R. Fasan, *Nat Chem*, **2017**, *9*, 609.

Two-Tier Screening Platform for Directed Evolution of Aminoacyl-tRNA Synthetases with Enhanced Stop Codon Suppression Efficiency. A. E. Owens; K. T. Grasso; C. A. Ziegler; R. Fasan, *ChemBiochem*, **2017**, *18*, 1109.

Metal Substitution Modulates the Reactivity and Extends the Reaction Scope of Myoglobin Carbene Transfer Catalysts. G. Sreenilayam; E. J. Moore; V. Steck; R. Fasan, *Adv Synth Catal*, **2017**, *359*, 2076.

Highly Diastereo- and Enantioselective Synthesis of Trifluoromethyl-Substituted Cyclopropanes via Myoglobin-Catalyzed Transfer of Trifluoromethylcarbene. A. Tinoco; V. Steck; V. Tyagi; R. Fasan, *J Am Chem Soc*, **2017**, *139*, 5293.

Ribosomal Synthesis of Thioether-Bridged Bicyclic Peptides. N. Bionda; R. Fasan, *Methods Mol Biol*, **2017**, *1495*, 57.

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Quantifying Early Time Quantum Decoherence Dynamics through Fluctuations. B. Gu; I. Franco, *J Phys Chem Lett*, **2017**, *8*, 4289.

Quantifying fermionic decoherence in many-body systems. A. Kar; I. Franco, *J Chem Phys*, **2017**, *146*, 214107.

Partial hydrodynamic representation of quantum molecular dynamics. B. Gu; I. Franco, *J Chem Phys*, **2017**, *146*, 194104.

When can time-dependent currents be reproduced by the Landauer steady-state approximation? R. Carey; L. P. Chen; B. Gu; I. Franco, *J Chem Phys*, **2017**, *146*, 174101.

Single-molecule force-conductance spectroscopy of hydrogen-bonded complexes. A. Pirrotta; L. De Vico; G. C. Solomon; I. Franco, *J Chem Phys*, **2017**, *146*, 092329.

Entanglement in the Born-Oppenheimer Approximation. A. F. Izmaylov; I. Franco, *J Chem Theory Comput*, **2017**, *13*, 20.

## ALISON FRONTIER

Diastereoselective Construction of Densely Functionalized 1-Halocyclopentenes Using an Alkynyl Halo-Prins/Halo-Nazarov Cyclization Strategy. G. Alachouzos; A.J. Frontier, *Angew. Chem. Int. Ed.* **2017**, *56*, 15030–15034.

## PENGFEI HUO

Coherent state mapping ring polymer molecular dynamics for non-adiabatic quantum propagations. S. N. Chowdhury; P. F. Huo, *J Chem Phys*, **2017**, *147*, 214109.

Ring Polymer Surface Hopping: Incorporating Nuclear Quantum Effects into Nonadiabatic Molecular Dynamics Simulations. F. A. Shakib; P. F. Huo, *J Phys Chem Lett*, **2017**, *8*, 3073.

Enhancing Singlet Fission Dynamics by Suppressing Destructive Interference between Charge-Transfer Pathways. M. A. Castellanos; P. F. Huo, *J Phys Chem Lett*, **2017**, *8*, 2480.

Excitation Energy Transfer in Light-Harvesting Systems: Theory, Models, and Application. P. F. Huo; D. F. Coker, *Ultrafast Dynamics at the Nanoscale: Biomolecules and Supramolecular Assemblies*, **2017**, 293.

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Aqueous Hydracity from Calculations of Reduction Potential and Acidity in Water. K. R. Brereton; S. M. Bellows; H. Fallah; A. A. Lopez; R. M. Adams; A. J. M. Miller; W. D. Jones; T. R. Cundari, *J Phys Chem B*, **2016**, *120*, 12911.

Synthesis, Characterization, and Reactivities of Molybdenum and Tungsten PONOP Pincer Complexes. R. Castro-Rodrigo; S. Chakraborty; L. Munjanja; W. W. Brennessel; W. D. Jones, *Organometallics*, **2016**, *35*, 3124.

Determination of Rhodium-Alkoxide Bond Strengths in Tp<sup>κ</sup>-Rh(PMe<sub>3</sub>)(OR)H. Y. W. Jing; Y. Z. Jiao; W. W. Brennessel; W. D. Jones, *Inorg Chem*, **2016**, *55*, 9482.

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Additive-Free Cobalt-Catalyzed Hydrogenation of Esters to Alcohols. Y. W. Jing; S. Chakraborty; W. W. Brennessel; W. D. Jones, *Acc Catal*, **2017**, *7*, 3735.

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Unexpected Solvent Effects in the Isomerization of (PCPIr)-P-iPr (eta(2)-PhC CPh) to a 1-Iridaindene. M. Wilklow-Marnell; W. W. Brennessel; W. D. Jones, *Isr J Chem*, **2017**, *57*, 968.

C(sp(2))-F Oxidative Addition of Fluorinated Aryl Ketones by (PCPIr)-P-iPr. M. Wilklow-Marnell; W. W. Brennessel; W. D. Jones, *Organometallics*, **2017**, *36*, 3125.

Catalytic oxidation of carbon monoxide by alpha-alumina supported 3 nm cerium dioxide nanoparticles. M. Wilklow-Marnell; W. D. Jones, *Mol Catal*, **2017**, *439*, 9.

Catalytic Dehydrogenative C-C Coupling by a Pincer-Ligated Iridium Complex. M. Wilklow-Marnell; B. Li; T. Zhou; K. Krogh-Jespersen; W. W. Brennessel; T. J. Emge; A. S. Goldman; W. D. Jones, *J Am Chem Soc*, **2017**, *139*, 8977.

## KATHRYN KNOWLES

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Tunneling in the Delayed Luminescence of Colloidal CdSe, Cu<sup>+</sup>-Doped CdSe, and CuInS<sub>2</sub> Semiconductor Nanocrystals and Relationship to Blinking. A. Marchioro; P. J. Whitham; K. E. Knowles; T. B. Kilburn; P. J. Reid; D. R. Gamelin, *J Phys Chem C*, **2016**, *120*, 27040.

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Uncovering active precursors in colloidal quantum dot synthesis. L. C. Frenette; T. D. Krauss, *Nat Commun*, **2017**, *8*, 2082.

Semiconductor quantum dot-sensitized rainbow photocathode for effective photoelectrochemical hydrogen generation. H. J. Lv; C. C. Wang; G. C. Li; R. Burke; T. D. Krauss; Y. L. Gao; R. Eisenberg, *P Natl Acad Sci USA*, **2017**, *114*, 11297.

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General and Efficient C-C Bond Forming Photoredox Catalysis with Semiconductor Quantum Dots. J. A. Caputo; L. C. Frenette; N. Zhao; K. L. Sowers; T. D. Krauss; D. J. Weix, *J Am Chem Soc*, **2017**, *139*, 4250.

PbSe quantum dot based luminescent solar concentrators. D. L. Waldron; A. Preske; J. M. Zawodny; T. D. Krauss; M. C. Gupta, *Nanotechnology*, **2017**, *28*, 095205.

Temperature-dependent optical properties of lead selenide quantum dot polymer nanocomposites. D. L. Waldron; R. Burke; A. Preske; T. D. Krauss; J. M. Zawodny; M. C. Gupta, *Appl Optics*, **2017**, *56*, 1982.

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# Staff News



*L to R: Pete Serrino, Jalil Shojaie, Sandip Sur, Bill Brennessel, Randi Shaw, Todd Krauss, Ted O'Connell, Barb Snaith, Val Fitzhugh, Evelyn Sucy-Caffery, Lynda McGarry, Donna Dolan, Anna Kuitem, Deb Contestabile, Gina Eagan, Doris Wheeler, Ken Simolo*

## 2017 Staff Retirements

Valerie Fitzhugh  
Dr. David Hickey  
Diane Visiko  
Marguerite Weston

## 2017 New Staff

Linda Boyle - Accounting Bookkeeper  
Robin Clark - Graduate Coordinator & Course  
Administrator  
Evelyn Sucy-Caffery - Secretary to Faculty



*Marguerite Weston and Donna Dolan*



*Donna Dolan, Evelyn Sucy-Caffery, Deb Contestabile*





Row 1: Diane Visiko  
 Row 2 (L to R): Gina Eagan, Donna Dolan, Barb Snaith, Randi Shaw, Todd Krauss, Robin Clark  
 Row 3 (L to R): Linda Boyle, Evelyn Sucky-Caffery, Anna Kuitems, Doris Wheeler, Deb Contestabile, Ken Simolo



Eric Lobenstine, David Hickey, Bruce Toder



L to R: Valerie Fitzhugh, Lynda McGarry, Deb Contestabile, Barb Snaith, Gina Eagan, Randi Shaw



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The department has established several funds that greatly benefit our departmental activities. Contributions from alumni and friends are the dominant source of income to these funds. If you wish to support the Department of Chemistry, please mark the appropriate box on the form below and send it with your contribution. Donations are tax-deductible; donations of appreciated securities may also carry significant tax advantages. If you wish to donate by credit card, please visit the website above. The chemistry department is grateful for your support.

## Chemistry Alumni Research Fund

A general fund that enhances the educational and research activities of the department. The fund enables a number of endeavors, among them Fellowship awards to support graduate research and education, the purchase of undergraduate laboratory equipment, assisting graduate students with travel expenses to scientific conferences, and supporting Chemistry's outside speakers program. Note that this fund is under direct control of the Department, and allows Chemistry to expand the scope of its research and teaching activities as needed. By contrast, the "Dean's Fund for Chemistry" is under control of the Dean of the College and not the Department, and is primarily used to supplant the College's expenses for ongoing Chemistry activities.

## Richard Eisenberg Chemistry Endowment

A new fund named to honor the distinguished career contributions of Richard S. Eisenberg, the Tracy H. Harris Professor Emeritus of Chemistry. Our goal with the fund is to endow a Chaired Professorship that can be used to attract a senior hire in the areas of inorganic chemistry, photoinduced charge transfer and/or photochemistry. In addition to allowing the faculty size to more rapidly grow to our new allotment, the Chaired Professorship position will allow us to build on current strengths in the Department in catalysis and photochemistry in order to nucleate larger, campus-wide research efforts in these areas.

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**LATEST NEWS** \_\_\_\_\_  
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