

# CHEMISTRY

# 2015-2016 Newsletter













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Lynda McGarry

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CHEMISTRY LIBRARIAN

Sue Cardinal

# **From the Chair**

Greetings to Chemistry Department students, faculty, staff and especially our alumni! I am thrilled to share with you some of the developments within Chemistry and the University during this past year, my fourth as Chair of the Department.

One of the true privileges of being on the faculty at Rochester is working with some of the most talented undergraduates in the world. This past May, we graduated 30 seniors who will pursue a variety of interests ranging from working in chemical companies around the country, to obtaining advanced degrees in biomedicine, chemistry and related STEM fields, to attending business school, to volunteering in science education related fields. Also, some graduates can't get enough of Rochester and are taking advantage of the Take-5 program to stay on campus for a 5<sup>th</sup> year. Going forward we will have close to 50 chemistry majors in the senior and junior classes this coming academic year, which is about our historical average.



Two new initiatives were started this year with respect to improving the undergraduate educational experience. First, we have expanded our efforts in hands-on experiential learning, pioneered by Chemistry faculty such as the late Jack Kampmeier. This past year, Professor Joe Dinnocenzo supported an exciting new venture to provide additional training for Workshop Leaders through the Kampmeier Workshop Fund. In collaboration with a local theatre-based training company, the Chemistry Department has begun to develop a program where we use theatre-based training to help Workshop Leaders from several academic departments learn how to better engage students in Workshops. Second, we have committed to a modernization of the junior level physical chemistry laboratories, CHM 231 and CHM 232. In particular, Professors Dave McCamant and Lewis Rothberg are adding more analytical chemistry experiments to CHM 231, and adding experiments in supramolecular and macromolecular chemistry, and nanoscience into the CHM 232 curriculum. These changes to laboratories will be phased in over the next few years as we successfully compete for grants that allow for the purchase of new equipment for the laboratories.

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! Two special mentions: I want to congratulate Astrid Olivares who won an NSF Graduate Research Fellowship this past year, and Valerie Fleischauer who won our recently endowed Outstanding Graduate Student Award. Our graduate program had an extremely busy year as 31 students have received their doctoral degrees since the Fall of 2015. Our total number of enrolled graduate students is currently at 87, along with 14 postdoctoral fellows. The Department welcomed a class of 20 new Ph.D. students in Fall 2016. 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 several potential new hires.

The Chemistry faculty continue to be recognized for their excellence in scholarship. In particular, we want to highlight the accomplishments of several faculty including Daniel Weix, who was named a Fellow of the AAAS this past year. Michael Neidig was one of 27 scientists from Universities to win a Department of Energy Early Career Award, and he also was honored with a chaired faculty position this year as well. Mike was named the Wilmot Assistant Professor of Chemistry, a title that is awarded every two years to the top Assistant Professors at the University! Although here for only a short time, Ellen Matson and Ignacio Franco both won CAREER awards from the National Science Foundation, which is impressive! Doug Turner won the Poland-U.S. Science

award sponsored by the American Association for the Advancement of Science (AAAS) and the Foundation for Polish Science (FNP). Finally, we are also proud of the dedication and effort that our faculty put into teaching at all levels. It is nice to see that work recognized from time to time, as it was this year when Brad Nilsson was awarded a 2016 Goergen Award for Excellence in Undergraduate Teaching.

One of my major goals for the Department for the near future is to lay the groundwork for the expansion in faculty size to 26 (from the current 20) over the next 5 to 7 year timeframe to significantly strengthen our research portfolio. Although the considerable costs associated with starting up a new faculty member in Chemistry have made accelerating faculty hiring challenging, we are still working with the College to turn this commitment into a reality sooner rather than later. We were encouraged that this year we were allowed to search for a faculty member in either synthetic organic, bioorganic, or biophysical chemistry. Should we be successful in the search it will push our faculty size to levels that we have not seen in Hutchison Hall in over two decades. Further, we are delighted to report that we are actively looking to fill the Andrew Kende Chair with an outstanding senior hire in synthetic organic chemistry. I hope to have more to report on our success in this venture in next year's newsletter! We have also made great progress on our goal of fully endowing the Richard Eisenberg Chemistry Fund, named to honor Rich Eisenberg, the Tracy H. Harris Professor Emeritus of Chemistry. Once fully vested, the proceeds from this fund will be used to help attract top caliber senior faculty to Rochester in the general areas of inorganic chemistry and/or photoinduced charge transfer and photocatalysis. Thanks to everyone who donated to the Kende and Eisenberg funds as your support is, and will continue to be, crucial to expanding the reach of the Department into novel areas of Chemistry research.

I want to thank all of our alumni for your continuing and generous support of the Department for the past year. Our "Chemistry Alumni Research Fund" is a great resource as it enables us to pursue a number of impactful endeavors, including being used this year to support almost two dozen Fellowship awards to support graduate 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.

I have enjoyed meeting some of you during my first term as Chair, and I sincerely hope to meet more of you during your visits to Rochester, or at one of the national ACS meetings over the next few years. Our chemistry alumni around the country provide critical input into how to best advance Chemistry at Rochester and we appreciate the discussions and the input. Finally, I wish to extend a personal invitation to return to Rochester for Meliora Weekend in 2017, with events running October 12<sup>th</sup> through the 15<sup>th</sup>. We will continue to have the annual Chemistry Department Gates Happy Hour on campus in the late afternoon on Saturday of Meliora Weekend. The Gates Happy Hour provides a special opportunity to get acquainted with current members of the Department and reconnect with old colleagues and classmates.

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

Sincerely,

Jul D. Hemes

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

# Donors 2015-2016

### JULY 1, 2015 TO DECEMBER 31, 2016

### GIFTS OF \$100,000+

Dr. Barbara J. Burger (B.S. `83) Dr. Dean C. Marvin (B.A. `73) and Laura Marvin

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- Dr. Linfeng Zie (M.S. 87, Ph.D. 90)
- Dr. Yang Zhao (M.S. 13, Ph.D. 15)



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

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#### **PROFESSOR ESTHER CONWELL**

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**DR. ALEXANDER L. JOHNSON** Dr. Joan E. Johnson (B.A. `64)

#### **PROFESSOR JACK A. KAMPMEIER** Dr. Richard English (B.S. `65) and Apita Wil

Dr. Richard English (B.S. 65) and Anita Whelan

#### **PROFESSOR NABI MAGOMEDOV**

Andrei Burnin and Irina Burnina Dagmara Magomedova Dmitry Zuev Larisa Zueva

**DR. ESTHER SPRENKEL-SEGEL** Dr. Ralph E. Segel

#### **DR. W. BERNARD WARGOTZ**

Laurie Block MBL Family Foundation Michael Wargotz





### JOHN AND DORIS BARG ENDOWED SCHOLARSHIP IN CHEMISTRY

John L. Barg and his wife Doris have established an endowed scholarship fund that will provide scholarship support for undergraduate students who are majoring in Chemistry.

John L. "Jack" Barg was born February 12, 1924 in Rochester NY. He grew up in Rochester, where his parents were from, and Jack's father owned a small cement construction business. Jack attended the University of Rochester from 1942 through 1946 and graduated with a degree in Chemistry. Jack loved to go over to the Sibley Library to study and listen to old jazz tapes. He has maintained his status as an Alumni member for over 70 years and has been a proud member of The George Eastman Circle.

After graduation, he was recruited by The B.F. Goodrich Rubber Company and came to Akron in 1946. He worked at Goodrich for about 2 years before moving on to take a position at The Barefoot Sole Shoe Company in Wadsworth, Ohio just outside of Akron. He worked there for 35 years before retiring.

Jack met Doris M. Guessford of Barberton, Ohio in 1949 and they were married on January 20, 1951. She worked for over 35 years at The Ohio Bell Telephone Company and then AT&T. Jack enjoyed listening to old great jazz artists of the 30's through the 60s and was an avid reader of the daily papers which he read from first page to last. He would stay on top of current events this way. At 92, he still reads the morning paper every day the same way. Jack and Doris were both avid euchre players, and Doris also loved to knit and play Mahjong in her later years. The hobby that they enjoyed the most was taking cruises together. They traveled by boat all over the world, and as Jack says, "We went through the Panama canal six times- three times from each direction!" Sadly, Jack's dear wife Doris passed away on February 9, 2015.

# CONTRIBUTIONS IN HONOR OF.....

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

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

### **PROFESSOR ANDREW S. KENDE**

Dr. Paul C. Naegely (M.S. `77, Ph.D. `79) and Stella Naegely

# MATCHING/ CORPORATE GIFTS.....

American Endowment Foundation Arnold & Mabel Beckman Foundation Chevron Corporation Dow Chemical Company ExxonMobil Foundation GlaxoSmithKline IBM Corporation Network for Good Pfizer Corporation, Inc. Shell Oil Company Foundation Texas Instruments Foundation Xerox Foundation/Xerox Co.

### FOUNDATIONAL

Leukemia & Lymphoma Society Schwab Charitable Fund Alfred P. Sloan Foundation MBL Family Foundation

### **NOT-FOR-PROFITS**

Fidelity Charitable Gift Fund Network for Good

### **GIFTS FROM CORPORATIONS**

Novartis Wyndham Worldwide Abbott Laboratories

### DEAN AND LAURA MARVIN ENDOWED SCHOLARSHIP FUND



Laura and Dean Marvin at the Grand Canyon (November 2016)

"I have chosen to establish the Dean and Laura Marvin Endowed Scholarship fund for two reasons. The first is to recognize the outstanding undergraduate education in Chemistry that the University of Rochester provided me. The preparation at UR allowed me subsequently to take full advantage of the PhD program in Physical Chemistry at UCLA and an industry postdoctoral position at IBM and Stanford University.

The second reason for this scholarship is in recognition that the UR education is not financially accessible to many high school graduates, some of whom might go on to make great scientific contributions given the

opportunity. The enthusiasm and skills for such a career are nurtured in the undergraduate years, and I would like to help someone reach as rewarding a career as I have had. The bulk of my career was spent at The Aerospace Corporation in Los Angeles, starting as a researcher and culminating as the Principal Director of the corporate Research and Development Program. Every day that position reminded my how important it is that the United States continue to produce great scientists whose work will drive the intellectual curiosity and economy of this country. This scholarship is my contribution to this goal."

# In Memoriam

### The Department of Chemistry mourns the passing of:

Barbara Ashton (B.A.`47) Dr. David A. Bittker (Ph.D.`53) Dr. Joseph F. Bunnett (Ph.D.`45) Dr. Jerald L. Connelly (B.S.`50, Ph.D.`58) Dr. Walter D. Conway (Ph.D.`56) Dr. Maria Rico Ferreira (Flw) Dwight E. Gardner (B.S.`46) Dr. Robert W. Hendricks (B.S.`51) Dr. Joseph W. Hickey (Ph.D`42) Dr. Alexander L. Johnson (Ph.D`64) Dr. Russell D. Johnson (B.S.`50) Pearl D. Klionsky (B.A.`46) Dr. Charles H. Klute (Ph.D. `42)
Dr. Philip L. Kumler (Ph.D. `68)
Ronald M. Levinson (B.S. `56)
Dr. Lefford F. Lowden (B.A. `63)
Dr. William C. Luft (B.S. `52, M.D. `56)
Dr. Robert A. Mooney (B.S. `55)
Dr. Geoffrey A. Page (Flw `53)
Dr. William H. Parsons (B.S. `72, Flw `80)
Dr. Dimitri Pyrros (B.A. `81, B.S. `81)
Dr. John M. Rutherford (Ph.D. `59)
Dr. Richard J. Windgassen (Ph.D. `59)
Alice M. Zawadzki (M.S. `68)



David A. Bittker (Ph.D.'53- W.D. Walters) (November 16, 2015) Dr. David A. Bittker attended Cornell University and the University of Rochester, receiving his Ph.D. in physical chemistry. This "rocket scientist" retired from NASA after 40 years of service at Lewis research center in Cleveland, Ohio.



Joseph F. Bunnett

Joseph F. Bunnett (Ph.D. '45- D. Stanley Tarbell) (May 23, 2015) Professor Emeritus Joseph F. Bunnett, a long-time member of the Department of Chemistry and Biochemistry at UC Santa Cruz, was one of the early builders of the department in the late 1960s and 1970s. He came to UC Santa Cruz in 1966 from Brown University and continued a distinguished career as one of the most nationally and internationally respected physical organic chemists, making his mark not only in publishing seminal papers in the area of organic reaction mechanisms, but also as an educator and leader. He was a founding editor of one of the top American Chemistry Society journals, Accounts of Chemical Research. His idea that a journal devoted to short, concise, and critical articles offering easy-to-read overviews of basic research in all areas of chemistry would be highly desirable proved to be visionary.

Joe received numerous honors in recognition of his many outstanding contributions to our understanding of chemical reactions. He was a Guggenheim Fellow, a Fellow of the Japan Society for the Promotion of Science, and twice a Fulbright Fellow. He is a Fellow of the American Academy of Arts and Sciences and of the American Association for the Advancement of Science. He was elected Honorary Member of numerous European and South American chemical societies, and he was the recipient of the 1992 James Flack Norris Award in Physical Organic Chemistry and the 1995 University of Rochester Distinguished Scholar Medal. After his retirement, Professor Bunnett focused on research related to the destruction of chemical weapons.



Walter D. Conway (Ph.D.'56 - D. Stanley Tarbell) (September 2015) Dr. Walter 1. D. Conway joined the SUNY University at Buffalo Department of Pharmaceutical Sciences in 1967 after working Dr. B.B. Brodie's in laboratory at the NIH.

He was granted tenure in 1971 and his position was expanded to a joint appointment with the Department of Medicinal Chemistry in 1975. Dr. Conway taught pharmaceutical chemistry and a course on the analysis of drugs in body fluids. He also taught an elective course on drug metabolites and drug metabolism until he retired in 2000. He continued as an emeritus professor maintaining some research activities in Kapoor Hall in advancing counter-current chromatography (CCC). His 1986 paper on this technique in *CRC Critical Reviews in Analytical Chemistry* remains among the most highly-cited in the field.



Alexander L. Johnson (Ph.D.'64-D.Stanley Tarbell) (November 16,2015) Dr. Alexander L. Johnson was born in Gisborne, New Zealand on October 13, 1931 and he moved to Wellington, New Zealand to attend Victoria University

earning his B.Sc. in Chemistry in 1953. One year later he earned his M.Sc. degree with first class honors. For the following five years he taught high school at Wellington's Rongotai College. In August 1960 Alex emigrated to the United States on a Fulbright grant to pursue a Ph.D. degree at the University of Rochester where he met his future wife Joan in the organic chemistry lab when he was her lab instructor. Under the direction of Professor Dean Stanley Tarbell he researched the chemistry of the antibiotic spectinomycin. He married Joan in 1961, and in 1964 he began a thirty year career in chemical research at DuPont and then DuPont-Merck Pharmaceuticals at the Experimental Station in Wilmington, Delaware. His research involved a broad series of projects on exploratory heterocyclic medicinal and plant growth regulatory efforts. He was the group manager of the cardiovascular research group that discovered Cozaar (losartan), the first of a new class of blood pressure

regulating drugs. At the time of his retirement in 1994 he was the Associate Director of Research at DuPont-Merck. He was also the author or coauthor of 105 publications, 14 patents, and speaker at numerous scientific meetings. Alex was an emeritus member of the American Chemical Society and a Fellow of the New Zealand Institute of Chemistry. He is survived by his wife Joan, three children, and five grandchildren. Award). His volunteer activities were many and varied including serving as treasurer of the SUNY day care center; volunteer at the Collins Correctional Visitors Center; Meals on Wheels deliverer; treasurer of the Darwin Barker library; and Treasurer and President of the Dunkirk- Fredonia Lions Club. Phil is survived by his loving wife and partner Rosemary (Bailen) Kumler, two children and five grandchildren.



Alexander and Joan Johnson



Philip L. Kumler (Ph.D. `68 - Marshall D. Gates, Jr.) (June 28, 2015)

Dr. Kumler was born May 23, 1941 in Columbus, Ohio. Philip received his B.A. in Chemistry from Miami University, and Ph.D. in Organic Chemistry from the University of Rochester working with Professor Marshall Gates. He held postdoctoral

research appointments at the University of Copenhagen (Denmark) and the University of Chicago. His first teaching position was at Saginaw Valley State College from 1970-1976. He then joined the Chemistry faculty at State University of New York at Fredonia as Associate Professor and Chair of the department (1976-1983). He was promoted to Full Professor in 1980 and retired in 2006 as Professor Emeritus. During his teaching career, he received the Franc A. Landee Award for Excellence in Teaching (Saginaw Valley), and the SUNY Excellence in Teaching Award in 1986. In 2006, he received the Chancellor's Award for Research and Scholarship from SUNY. In October 2014, he was honored with the naming of the Kumler Spectroscopic Instrument Room at the new science center on the Fredonia campus, funded by several of his previous students. A scholarship fund has also been established in his name (The Senior Seminar



William C. Luft, M.D. (B.S.'52, M.D.'56) (August 28, 2016) Dr. Luft was born in Goshen, N.Y., on Jan. 25, 1931. He was an Eagle scout, and graduated from Goshen High School, where he won the Bausch & Lomb Honorary Science Award. This award resulted in a scholarship to

the University of Rochester, where he earned his B.S. and M.D. After his internship at Rochester's Strong Memorial Hospital, he performed his surgical residency at Genesee Hospital, followed by his service in the U.S. Air Force, in which he was a flight surgeon. He did his anatomic pathology residency at Boston City Hospital and then his clinical pathology residency at University of Minnesota in Minneapolis, Minn. He was an assistant pathologist at Genesee Hospital in Rochester, N.Y., before joining the team at Robert Packer Hospital and Guthrie Clinic as an assistant pathologist in 1967. He was named co-chair of the department in 1970 and remained there until his retirement. He was a member of several professional organizations, including the American Society of Clinical Pathologist, College of American Pathologist, American Association of Blood Banks, and the American Association for Clinical Chemistry. His motto was "Please Give Blood" and he had given 17 gallons of blood over the course of his lifetime. Bill is survived by his wife Carolyn, five children and several grandchildren.

William H. Parsons (B.S. '72, Flw'80) (June 11, 2016) Dr. Parsons, 66, received degrees in chemistry from the University of Rochester and the University of Vermont. He was a senior research director in pharmaceuticals at Merck and Johnson & Johnson. He was an avid outdoorsman and enjoyed vacationing and fishing in Maine. Burial was at Pine Hill Cemetery in Rush, N.Y.



Morris J. Shapiro (B.A. '34, M.S.'34) (February 25, 2016)

A native Rochesterian, Dr. Shapiro was born Oct. 21, 1913. Dr. Shapiro was the oldest active faculty member at the University of Rochester Medical Center. He received a full scholarship and attended the University of Rochester in the first

class on River Campus. He graduated Phi Beta Kappa in just three years with a bachelor's degree in Biology in 1933, using his fourth year to earn a master's degree in Chemistry. He went on to attend medical school at Jefferson Medical College in Philadelphia, graduating in 1938.

He began practicing medicine as a military surgeon in the U.S. Army during World War II, serving in Africa and Italy. He led the surgical team of the 16th Evacuation Hospital in Northern Africa and Italy. It was during the war that Dr. Shapiro met his wife, Miriam, who was a nurse serving on a ship sent to support the Allied troops. When her ship was sunk off the Italian coast, she and the surviving nurses rowed ashore and went ahead and set up their hospital. After the war, Mrs. Shapiro taught biology at the University of Rochester and maintained incredible scientific interests that included many travels. Dr. Shapiro worked at Rochester General, Genesee and Strong Memorial hospitals. He established Rochester's first free clinic for the early detection of breast cancer. He served as a general surgeon in the URMC Department of Surgery until his "retirement" 30 years ago, when he began work in Emergency Medicine, practicing and teaching through January of 2016.

In celebration of his 100th birthday, Dr. Shapiro created the endowed Miriam F. and Morris J. Shapiro M.D. Resident Growth and Education Award, given to residents who exemplify a passion for learning and a dedication to growth in the knowledge of the Emergency Department. Predeceased by his wife Miriam in 2003, Dr. Shapiro is survived by his daughters, Donna and Barbara, and his grandchildren, Jessica, Marissa and Kate.



### Esther Sprenkel-Segel (Ph.D.`59- Edwin O. Wiig) (September 29, 2016)

Dr. Sprenkel-Segel was born in 1931 and raised in York, PA where she served as valedictorian of her class at William Penn Senior High School and returned regularly for reunions. She went on to major in math

at Goucher College and earn a doctorate in nuclear chemistry from the University of Rochester. She and husband, Dr. Ralph E. Segel, met at Brookhaven National Laboratory on Long Island, where she did her thesis research with the Nobel laureate Professor Raymond Davis, Jr. Her career continued at Argonne National Lab and on the faculty at the Illinois Institute of Technology. Esther lived a long and full life. She enjoyed 56 years of marriage with Ralph in Wilmette, Illinois. They had three children, Dan, Ginger and Tanya; and nine grandchildren, who were her pride and joy, Sophie, Harry, Alex, Peter, Oscar, Charlie, Owen, Elle and Tate.



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

## **Alumni News**



Dr. Clifford P. Kubiak (Ph.D.`80), Harold C. Urey Chair and Distinguished Professor of Chemistry & Biochemistry at the University of California, San Diego, is the recipient of the 2015 Fred Basolo Medal in recognition of his work in inorganic chemistry. The award is given by Northwestern University and is cosponsored by the

ACS Chicago Section. It is named for late Northwestern chemistry professor Fred Basolo. Kubiak's research is in catalytic transformations of  $CO_2$ , artificial photosynthesis, ultrafast electron transfer within the ground states of inorganic mixed-valent systems, and theoretical and experimental investigations of electrical conductivity of molecular assemblies. He presented a lecture during a local section meeting at Northwestern in October 2015. In April of 2014, Kubiak was elected a member of the American Academy of Arts and Sciences.

Kubiak received a Bachelor of Science degree with honors in chemistry from Brown University in 1975 and a Ph. D. in Chemistry from the University of Rochester in 1980, where he worked with Richard Eisenberg. Kubiak was a postdoctoral associate with Mark S. Wrighton at M. I. T. from 1980-81. From there, Kubiak went on to be a faculty member at Purdue University from 1982 – 1998. He moved to UCSD in 1998 as Harold C. Urey Endowed Chair Professor and was named Distinguished Professor at UCSD in 2008.

Dr. Kubiak has also served as the Faculty Athletics Representative for UC San Diego's Department of Intercollegiate Athletics since 2007. A distinguished professor of chemistry and biochemistry at UCSD, Kubiak serves as a liaison between the institution and the athletics department, and also as a representative of the institution in conference and NCAA affairs. Kubiak also chairs the Faculty Athletic Board of Advisors (FABA). In June of 2013, Kubiak received the Athletics Department's Meritorious Service Award.



Fred Lewis speaking at Bill Sanders 90th birthday gathering

**Dr. Frederick D. Lewis (Ph.D.'68),** professor of chemistry at Northwestern University was selected to receive the 2015 Josef Michl ACS Award in Photochemistry for his elegant, incisive research on the photochemistry of molecules from ketones to DNA, and his mechanistic analyses that explain, clarify, and generalize these experimental results. In May 2016, Dr. Lewis was also awarded The Porter Medal, named for the late George Porter FRS, Nobel Laureate, which is given biennially to the scientist who, in the opinion of the European Photochemistry Association, the Inter-American Photochemistry Society, and the Asian and Oceanian Photochemistry Association, has contributed most to the subject of Photochemistry.

After receiving his training at Amherst College, Rochester (with William H. Saunders, Jr.), and Columbia (Nicholas J. Turro), he joined the faculty at Northwestern University in 1969. For the past two decades Dr. Lewis and his collaborators have investigated the dynamics and mechanism of photoinduced injection and transport of positive and negative charge in synthetic DNA hairpins using a combination of molecular design, ultrafast spectroscopy, and theory. Dr. Lewis is also a fellow of the AAAS and the ACS, and an Arthur C. Cope Scholar.



Reflections from Dr. Ray Carman (FLW`57) "I did my BSc, MSc and PhD degrees in Wellington, New Zealand. All my teachers were European-trained, mostly Oxford or Cambridge, and it was considered that

that was where I should post-doc. Certainly there were useful contacts there. But I was reading J. Amer. Chem. Soc., and J. Org. Chem., and good science was coming out of the USA, so I decided to venture there. But where? Rochester, with Stan Tarbell, Bill Saunders, Marshall Gates (who had just synthesized morphine) and Virgil Boekelheide, presented a formidable organic team. But where was Rochester? No internet in those days, but 'The World of Learning' was available as a large tome in the Wellington library. I did a search of USA Universities, especially looking at library size, and found that UR had a formidably large one. And that it was the current home of the editorship of J. Amer. Chem. Soc. (Marshall Gates), so I decided it couldn't be a bad place. I applied out of the blue in 1957 to Stan Tarbell and was accepted (by snail mail, of course).

I attended the graduate seminars (6pm, the possibility of free beer and/or pizza) of Gates and Boekelheide, and turned my attention to the structure of fumagillin. Here I was extremely lucky. The first NMR machine that I, and most other people, had ever seen was delivered to the Department on Christmas Eve, 1958. There was some delay as it had been simply poured off the back of a truck, and the University was reluctant to accept it in damaged condition, but it was soon up and running. Perhaps 20 man-years (yes man- in those days!) of research had gone into the structure of fumagillin, and co-worker Derek Chapman and I had ~20 derivatives to examine. We knew nothing about NMR, but soon learned some principles - spread out the large printouts (each ~one meter long) all over the floor and look for similarities and differences. About midnight one evening in early 1959, I decided that one methyl group in  $\beta$ -hexahydrofumagillin, formed by LiAlH4 reduction of fumagillin, was a doublet, which we had never seen before elsewhere, and that it was at lowish field, suggesting a Me-CHOH- system, and I realised that this should give a positive iodoform test. Yes it did! Unique; no other fumagillin derivative gives this test. I performed the same test before Derek and Stan the next day, and we realised that the hydride had opened a C-C bond, and that we had essentially solve the fumagillin structure.

I returned to New Zealand, applied in 1960 for a lecturing position at the University of Brisbane, in Queensland, Australia, when Stan Tarbell's reference obviously served me well. I served there for 40 years, and remain an Honorary Fellow, still researching the avocado antifungal/antibacterial."

Dr. Valerie Kuykendall (Chandler) (Ph.D.'89) attended Rochester's Oscar Gala in February 2016 at the Kodak Center for Performing Arts where \$20,000 was raised to benefit the American Heart Association. The guests were entertained by the University of Rochester's own all-male a cappella group, the Yellowjackets! Valerie has worked in research at Eastman Kodak since receiving her doctoral degree with advisor Bill Jones, and is currently a Senior Ink Development Chemist. Valerie's daughter, Candace, was chosen to be Miss New York USA in 2014 and participated in the Miss USA competition. She works as a model and owns ThreeSixty Model Placement, an agency for models in LA. At St. John Fisher College, she became the president of the dance team and graduated magna cum laude earning a bachelor's degree as a double major in finance and accounting.



Valerie Kuykendall and Kodak CEO Jeff Clarke



Candace Kuykendall being crowned Miss New York 15

### **Saunders 90th Birthday**



The Chemistry Department celebrates 90<sup>th</sup> Birthday of Professor Emeritus William H. Saunders, Jr.

The Chemistry department faculty and some special guests gathered together on Thursday, August 1, 2016 at the Next Door Bar and Grill in Pittsford to celebrate the 90th birthday of Professor Bill Saunders that was on January 12, 2016. Joining the faculty were Bill's two children, Anne and Claude Saunders, and former doctoral students Dr. Fred Lewis and Dr. Karen Hill Brown. Fred Lewis (Ph.D. '68) has been a professor at Northwestern University since 1969, and was recently honored with the 2016 Josef Michl ACS Award in Photochemistry. Karen H. Brown (Ph.D. '72) was appointed Deputy Director of the National Institute of Standards and Technology, Department of Commerce after climbing the ranks as a manager at IBM specializing in the area of lithography, and is recently retired. Professor Joe Dinnocenzo emceed the event and introduced Fred and Karen, who told some great stories from their graduate school days. Anne and Claude Saunders also shared some stories from their childhood and what it was like having Bill as a father. It seems that he was a big Monty Python fan and passed it on to his children.





Bill with Karen Hill Brown and Fred Lewis



Bill with daughter Anne and son Claude









### Faculty Grants & Awards

### GRANTS

### Chemistry faculty to receive over seven million dollars in new and renewed funding:

### Lianping Xing (URMC), Robert K. Boeckman, Jr. (NIH) Protein modification in bone cell regulation (\$202K over 2 years)

The National Institute of Arthritis and Musculoskeletal Skin Diseases (NIAMS) has awarded an and Exploratory/Developmental grant (R21) to fund the research of URMC Professor Lianping Xing and Professor Robert K. Boeckman, Jr. for their work on finding a new and improved version of Velcade. Bone fractures affect a million Americans each year and we found that a drug called Velcade, used in the treatment of patients with multiple myeloma, can promote the healing of bone fractures in mice. However, Velcade has toxic side effects when it enters the bloodstream, limiting its broader use. Their proposal will study a new form of Velcade which will only act on bone, thereby reducing the side effects. If successful, their study will provide a new drug for patients with fractures and other bone-related diseases such as multiple myeloma, tumor metastasized to bone and osteoporosis.

# Rudi Fasan (NSF) SusChEM : Cytochrome P450 based catalysts for $C(sp^3)$ -H amination (\$333K over 3 years)

With this award, the Chemistry of Life Processes (COLP) Program in the Chemistry Division of the NSF is funding the Fasan group to develop and investigate enzymes (biological catalysts) that convert carbon-hydrogen (C-H) bonds into carbon-nitrogen (C-N) bonds. Carbon-nitrogen bonds are common in both man-made and naturally occurring organic molecules. Currently available methods for making C-N bonds from C-H bonds largely rely on the use of rare and expensive metals and wasteful reagents. Catalytic methods for the construction of C-N chemical bonds are potentially extremely valuable for the manufacture of commodity chemicals and pharmaceuticals. This project is developing enzymes that increase the rate of new C-N bond formation starting from easily accessible, low or zero waste raw materials. Since these chemical reactions do not occur in nature, this research has broad and farreaching implications toward expanding the range of synthetically-valuable chemical reactions.

### Ignacio Franco (NSF) 2016 Faculty Early Career Development (CAREER) Award - Decoherence, Non-Equilibrium Properties and Stark Control of Electrons at the Nanoscale. (\$625K over 5 years)

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. Using this award, Professor Ignacio Franco and his research group will investigate the fundamental limits in the laser control of electrons and electronic properties in matter by exploiting quantum mechanical effects, an area of research known as quantum control. The reason to focus on lasers over more conventional means (e.g., an applied voltage, or changes in thermodynamic control variables) is that lasers offer the possibility of dynamic manipulation on an ultrafast timescale (on the order of a millionth of one billionth of a second).

### Alison Frontier (NSF) Cascade cyclizations for small molecule synthesis (\$470K over 3 years)

The Chemical Synthesis Program of the NSF Chemistry Division supports the research of Professor Alison Frontier and her group who are developing highly efficient cyclization reactions which are capable of creating compact polycyclic molecules that are difficult to prepare using other synthetic strategies. These chemical methods enable rapid synthesis of complex natural and non-natural bioactive molecules, especially small molecules with properties demonstrated to be valuable in drug discovery efforts. With respect to educational activities, development continues for an educational website ("Not Voodoo"), which is designed as a resource for students beginning independent research in an organic chemistry laboratory.

### Todd D. Krauss (NSF) Synthesis, Synthetic mechanism, and Single Particle Microscopy of Colloidal Semiconductor Nanocrystals (\$450K over 3 years)

In this project funded by the Macromolecular, Supramolecular and Nanochemistry (MSN) Program in the Division of Chemistry, the Krauss group is studying tiny inorganic particles called colloidal semiconductor nanocrystals (NCs). These NCs have the potential to impact numerous areas of active research and technology due to their size-dependent properties. However, the lack of a rational synthetic mechanism has impeded advances in NC design and applications. This project investigates new fundamental strategies for low-temperature NC syntheses that are potentially scalable to industrial volumes, and thus are compatible with current chemical manufacturing procedures. Largescale synthesis of semiconductor NCs, especially those with reduced toxicity, may enable the development of new applications in biology and medicine, optics and photonics.

### Michael L. Neidig (NSF) 2015 Faculty Early Career Development (CAREER) Award- Iron- and Cobalt-Catalyzed Direct C-H Functionalization (\$675K over 5 years)

The Chemical Catalysis Division will support Professor Neidig's research on pursuing a detailed molecular understanding of the reactions in which carbonhydrogen bonds are broken and other molecules replace the hydrogen atoms. Neidig will also use part of the grant money to develop educational outreach programs in the Rochester community, including lab experiences for high school students and a short course for the Upward Bound program at the University designed to inspire underrepresented students to pursue careers in STEM.

### Michael L. Neidig (DOE) 2016 Early Career Award-Electronic Structure, Bonding, and reactivity in f-element Chemistry (\$750K over 5 years)

Michael Neidig was one of 49 scientists to be recognized in June 2016 by the Department of Energy as one of the nation's "exceptional researchers" in his or her "crucial early career years." Neidig will use the grant to study the electronic structure and bonding in lanthanides and actinides, including short-lived and transient molecules. Actinides, which include uranium, are particularly important in nuclear energy and nuclear nonproliferation. Lanthanides are important in the manufacture of semiconductors, hybrid car components, and glasses, among other products.

### Lewis J. Rothberg (NSF) Photophysics and stability of multichromophoric polyelectrolytes (\$285K over 3 years)

The NSF Division of Materials Research (DMR) has awarded funding to Professor Lewis Rothberg for research on a class of water-soluble polymers that are capable of light emission. The materials are being studied in collaboration with chemists who are

developing them for biomedical imaging of tumors, and for applications to detection of proteins and DNA sequences of medical interest. These polymers organize into geometries that are determined by factors such as salt and acid concentrations in the water. Those geometries strongly influence both the color and brightness of the light emitted from the polymers. The project employs microscopy of single polymer strands to investigate how the polymer conformation and solution conditions affect the intensity and stability of the emitted light.

# Daniel J. Weix, Todd D. Krauss (ACS-PRF New Directions) Homogeneous Colloid Catalysts for Visible Light Photochemistry (\$110K over 2 years)

The ACS PRF New Directions grants program is designed as a source of funds for new concepts and new projects. Principle investigators Daniel Weix and Todd Krauss will pursue a joint research effort to establish heterogeneous colloidal photocatalysts as a new, important class of photocatalysts that offer particular advantages for longevity, tunability, and sustainability. Efforts to calibrate the reactivity of the colloidal catalysts to known catalysts should speed up use in the wider synthetic community. In addition, we anticipate that our optimized catalysts will be simple to synthesize and will be made available from commercial suppliers.





Renewed funding for successful projects:

The Chemical Structure, Dynamics, and Mechanism B (CSDM-B) Program of the NSF has renewed funding for "Novel Cation Radical and Exciplex Chemistry," a proposal of Professor Joseph P. Dinnocenzo to investigate the selective formation of highly reactive aryl radicals under mild conditions. The grant provides \$570,000 over a three year period. The mechanistic insight gained from these studies can provide the knowledge necessary to rationally utilize the chemistry in synthesis and in the design of new materials. In addition, research on newly discovered cationic exciplexes and exciplexes that exhibit dual emissions will provide knowledge on these novel excited state intermediates. Student co-workers will learn to carry out chemical synthesis and to conduct mechanistic studies in photochemistry including a range of less traditional techniques (fluorometry, transient absorption spectroscopy, time-correlated single photon counting, electrochemistry, and modern computational methods).

Professors Kara Bren, Todd Krauss, and Richard Eisenberg have been awarded renewed funding of more than one million dollars for their DOE Single-Investigator and Small Group Research (SISGR) grant proposal entitled "Modular Nanoscale and Biomimetic Assemblies for Photocatalytic Hydrogen Generation". The overarching objective of this proposal is the development of systems to convert light energy into the formation of H2. For this project, nanocrystalline semiconductor particles will be synthesized that have size-dependent, quantum-confined properties. These nanoparticles will be engineered to harvest solar energy and efficiently separate electrons from positive holes. Molecular and biomolecular proton-reducing catalysts incorporating Earth-abundant metals will be integrated with the nanoparticles to form photocatalytic systems for converting light energy to H2 fuel from aqueous protons.

The Department of Energy has renewed funding for the promising research of Professor and Chair of the Chemistry Department Todd Krauss for \$435,000 over the next three years for the proposal "Photophysics of Charged Excitons in Single-Walled Carbon Nanotubes." Solar energy is very attractive as an alternative source of energy since it is renewable, carbon-free, and abundant. However, making solar energy competitive with carbon-based energy requires significant fundamental breakthroughs in solar energy harvesting efficiencies and in solar energy storage. Single walled carbon nanotubes (SWNTs) have several characteristics that make them highly attractive for future light harvesting, charge transfer and charge transport applications. SWNTs absorb strongly at near infrared wavelengths not absorbed by conventional Si based materials, are excellent conductors and electron acceptors, and are chemically and photochemically extremely robust. This project puts a major emphasis on studies of the photophysics of carbon nanotubes doped with electrons or holes. This line of research has

direct relevance for understanding how photoinduced charge carriers interact with existing charges on NTs, and thus how NTs will behave as possible components of light harvesting systems.

The DOE has renewed support for the research of Professor **William D. Jones** for his continuing studies of catalysis for the proposal "*Transition Metal Activation* and Functionalization of Carbon-Hydrogen and Carbon-Carbon Bonds" which will provide \$440,000 of support for three years. This ongoing project is directed towards fundamental investigations of the reactions of homogeneous transition metal complexes with aliphatic and aromatic hydrocarbons, saturated and unsaturated, and their functionalized derivatives. The Jones research group will also be supported by a NSF center grant "Center Enabling New Technologies through Catalysis (CENTC)" of \$406,000 for one year.

Professors **David McCamant** and **Richard Eisenberg** have also been awarded renewed funding for their NSF collaborative proposal with Professors **Michael Detty** and **David Watson** at the University at Buffalo on "*The Design, Chemistry and Study of Systems for Making Solar Hydrogen.*" The grant provides \$440,000 over a three year period. Abundant, environmentally benign energy for sustainable development is one of this century's great scientific and technological challenges. Hydrogen has been called the fuel of the future, but it will only fulfill that promise if it is produced using solar energy. This proposal offers an innovative approach to produce H2 from water using visible light. The proposed research contributes to fundamental science on which future solar energy technology can be developed and will generate understanding of system components and steps in the photogeneration of H2 using visible light and a molecular photo-catalytic system. Despite proofof-concept studies, the need for highly active and robust systems remains.

Professor Daniel J. Weix and his group have been awarded renewed funding of \$1.3 million over 4 years by the National Institutes of Health to develop new reductive cross-electrophile coupling reactions and study their mechanisms. Cross-electrophile coupling reactions were pioneered in the Weix group and are now frequently used at pharmaceutical companies in drug discovery and development. The specific aims of the proposal entitled "Cross-Coupling Without Organometallic Reagents: New Electrophiles, Reactions and Mechanisms for Cross-Electrophile Coupling" are to: (1) dramatically expand the number of electrophiles that can participate in radical-mediated cross-electrophile coupling and to further study the reactive intermediates in the proposed mechanism; (2) study a new mechanistic model for crosselectrophile coupling, multimetallic cross-electrophile coupling, and develop new cross-electrophile couplings of electrophiles that do not as easily form carbon radicals; and, (3) discover and study new ligands for cross-electrophile coupling through both mechanismguided design and the screening of novel ligand libraries.



### AWARDS

The James P. Wilmot Distinguished Assistant Professor of Chemistry, Michael L. Neidig, was named a 2015 Alfred P. Sloan Research Fellow, one of only 23 early career researchers in the field of Chemistry in the U.S. Professor Neidig's research focuses on non-precious metal catalysis in organic chemistry, including iron-catalyzed cross-coupling and iron- and cobalt-catalyzed direct C-H functionalization. To qualify, candidates must first be nominated by their fellow scientists and are subsequently selected by an independent panel of senior scholars. Each fellow receives \$50,000 over two years to help further his or her research.

Chemistry Professor Bradley Nilsson has been selected to receive the 2016 Goergen Award for Excellence in Undergraduate Teaching. The award was presented at a special award ceremony in the Hawkins Carlson Room located in Rush Rhees Library just before Meliora Weekend to Brad and two other faculty members, Beth Jörgensen (Spanish) and Amy Lerner (BME). Kelsev Tuttle (B.S. 16) gave a heartfelt and inspiring introduction for Brad at the ceremony. The award recognizes Professor Nilsson for his excellence in teaching the first semester undergraduate organic chemistry laboratory courses (CHM 173 and CHM 207), and the second semester organic chemistry lecture courses (CHM 172 and CHM 204). He also developed a graduate level course in Bioorganic Chemistry and Chemical Biology (CHM 440); advanced undergraduate students account for 84% of student enrollment. Along with classroom performance, the award recognizes innovation in course design and curriculum, teaching methods and style, integration of research and teaching, and the ability to create a rigorous and relevant environment in the classroom, where students of all abilities and experiences with chemistry are stimulated and challenged.



Established in 1997 by University Trustee Robert Goergen and his wife, Pamela, the Goergen Award for Excellence in Undergraduate Teaching recognizes the distinctive accomplishments and skills of individual teachers in undergraduate courses in the College.

Bradley Nilsson pictured with Kelsey Tuttle ('16)



Congratulations to **Douglas** Turner, professor of chemistry, who, with his collaborator **Ryszard** Kierzek, a professor at the Institute of Bioorganic Chemistry Polish Academy of Sciences in Poznan. has received the Poland -U.S. Science Award from the American Association for the Advancement of Science (AAAS) and the

Foundation for Polish Science. The award, established in 2013 and given once every two years, honors their collaboration of more than 30 years investigating the thermodynamics, biology, and structure of ribonucleic acid (RNA) and RNA chemical synthesis. Because of their work, AAAS says, it is possible to predict the structure of any RNA based on its sequence. Their research also elucidates RNA folding rules and the use of modified oligonucleotides to modulate biological activity of pathogenic RNAs, such as inhibiting the growth of the influenza virus. The parameters that Doug developed, known as "Turner Rules," allow for the prediction of RNA folding. He has published more than 230 scientific articles, cited more than 15,000 times.

**Daniel Weix**, associate professor of chemistry, has been named a **Fellow** of the **American Association for the Advancement of Science (AAAS)**, the world's largest general scientific society. Election as an AAAS fellow is an honor bestowed upon AAAS members by their peers. "AAAS is one of the most outspoken organizations on behalf of all of science worldwide, so it's exciting to be recognized by an organization like that," he says. Weix is a specialist in organic (carbonbased) synthesis. He works on developing better ways of creating molecules in order to accelerate the discovery of new, useful compounds. Weix's citation is for distinguished contributions in the area of practical metal-catalyzed cross-electrophile coupling reactions.



### Seed money for new research directions from the University:

Rudi Fasan, Associate Professor of Chemistry; Danielle Benoit, Associate Professor of Biomedical Engineering; and Benjamin Frisch, Research Assistant Professor of Medicine (Hematology/Oncology) were recipients of a 2016-17 University Research Award. Their proposal, "Targeted Delivery of Cytotoxic Agents for the Eradication of Leukemia Stem Cells in the Bone Marrow", was one of eight applications chosen by senior research leadership. It is described as an initial assessment of the functionality and therapeutic potential of developing a novel nanoparticle-based system for the controlled and selective delivery of antileukemic agents to acute myeloid leukemia and leukemia stem cells within the bone marrow. The University Research Awards provide seed money on a competitive basis for innovative research projects that are likely to attract external support when sufficiently developed.

Chemistry faculty members are co-investigators on two of the four teams that have received the latest round of awards from the **University's Technology Development Fund**. TDF funding allows for proofof-concept experimentation and pre-clinical studies. **Prof. Rudi Fasan** is working with Prof. Lynne Maquat (Biochemistry and Biophysics) with the intent to design, develop, and test inhibitor compounds that will permeate and silence breast cancer cells. **Prof. Robert Boeckman** and **Dr. Frank Ebetino** seek to engineer a tissue-selective extension of known therapeutic compounds in order to cause effective drugs to adhere to human bones.

The October **2015 PumpPrimer II award** winners included the four Chemistry faculty members listed below. Pump Primer awards were created to help faculty gather preliminary data in order to seek extramural funding for "bold new research directions." The awards, available to Arts, Sciences and Engineering researchers through the Dean's Office, are typically in the \$20,000 range for one year, and can make all the difference in keeping a promising line of research alive.

**Kara Bren:** "Engineered Biomolecular CO<sub>2</sub> Reduction Catalysts."

**David McCamant:** *"Ultrafast Laser Spectroscopy of Molecular Exciton Dynamics."* 

**Todd Krauss** and **Daniel Weix:** "A Novel, Non-Classical Light Source: Syntheses and Characterization of Optically Active Defects in Glass."



### **COR-ROC Inorganic Chemistry Symposium**









On Saturday April 9th, 2016 the first Cornell-Rochester Inorganic Symposium was held at the University of Rochester. The event, organized by Prof. Ellen Matson from the University of Rochester and Prof. Justin W. Wilson from Cornell University, focused on facilitating collaboration and discussion between the inorganic research groups between the two departments. Four graduate students and postdoctoral researchers from each university were selected to give a 20-minute research talk. In addition to these eight research talks, twenty-four research posters were presented by students and postdoctoral researchers from research labs in both departments. The keynote speaker was Professor Emeritus Rich Eisenberg on "Fuel from Water: The Light-Driven Generation of Hydrogen."

Given the success of the inaugural event, we plan to extend this symposium to the Chemistry Departments at Syracuse University and the State University of New York at Buffalo in 2016. This year's mini-conference entitled the *Western New York Inorganic Symposium* will be held on June 3<sup>rd</sup> in Ithaca, New York.



### **CBI Retreat**

### Materials Science Symposium



The Biological Chemistry Cluster hosted its annual retreat May 19-20, 2016. The goal of the retreat is to stimulate interactions among faculty, postdocs, and graduate students across campus with interests in research at the interface between chemistry and biology. The retreat also aims to raise awareness on campus about research at the

forefront of the field more broadly. This year, the retreat again saw wide participation, with 80 attendees from the Departments of Chemistry, Biology, Biochemistry & Biophysics, Microbiology, Pharmacology & Physiology, Biomedical Engineering, and Dermatology. The retreat was made possible with the generous support of the University Committee for Interdisciplinary Studies (UCIS), and the Department of Chemistry.

The featured speaker at this year's retreat was Prof. Tom Kodadek, Chair of Cancer Biology and Professor in the Department of Chemistry at The Scripps Research Institute (Florida Campus). Prof. Kodadek gave an outstanding talk on "Chemical Tools to Monitor and Manipulate the Proteome" that highlighted the role that chemical biology plays in translational science. The next day, the retreat continued at the Staybridge Suites Hotel with 80 attendees. Another highlighted visitor who spoke was Prof. Brian Callahan of SUNY Binghamton, whose talk was on "Proteins on Steroids: Biochemistry of a Forgotten Lipidation Event." This excellent talk highlighted the exciting work that can be done in a University department where the PIs rely primarily on undergraduate researchers. Both Prof. Callahan and Prof. Kodadek participated in a lively career panel along with Dr. Cecilia Barone of the Center for Excellence in Teaching and Learning and Dr. Calvin Uzelmeier of the Rochester Museum and Science Center. After a lunch buffet and poster session, the retreat concluded with short talks from Jen Urban (Krauss and Nilsson groups), Josh Dewe (Fu group, UR BIology), Kathy Clark (Dumont group, UR Biochemistry & Biophysics), and Letty Salas-Estrada (Grossfield group, UR Biochemistry & Biophysics).

The retreat saw many new connections made and that enhance research and training at the Chemistry-Biology Interface at UR. Students, postdocs, and faculty gained a greater awareness of the breadth of research done at UR in this exciting area, and everyone greatly enjoyed the interactions with our distinguished visitors. We look forward to hosting the next retreat in 2017.

On Monday May 16, 2016, the Rochester Advanced Material Program(RAMP) hosted the annual Frontiers in Materials Science for the 21st Century one day symposium on the topic of "MEMS and Membranes" at Sloan Auditorium at the University of Rochester. The symposium was organized by Dr. James McGrath(BME) and Dr. Kara Bren(Chemistry). Gina Eagan, administrative assistant for the Materials Science program, took care of all of the logistics. Porous membranes are used ubiquitously as filters, barriers, and interfaces. The advent of nanotechnology has provided new materials and tools for the design of membranes that are far more precise and efficient than the conventional haphazard assembly of polymers. The presentations followed the "Gordon Conference" format, where a significant proportion of time is reserved for discussion and exchange of ideas. More information about the UR Materials Science program can be found at: https://www.rochester.edu/college/matsci/index. html.

Keynote speakers included:

#### Shigeru Amemiya, Univ. of Pittsburgh

"Nanoelectrochemical Study of Molecular Transport through Biological and Artificial Nanopores"

#### Thomas Gaborski, RIT

"Ultrathin Transparent Membranes for Cellular Barrier Models"

Jirachai Getpreecharsawas, Univ. of Rochester "Porous membranes as pumps"

Jeffrey Gralnick, Univ. of Minnesota "Harnessing Extracellular Electron Transfer for Biocatalysis"

#### Bruce J. Hinds, Univ. of Washington

"Dramatic nano-fluidic properties of carbon nanotube membranes as a platform for protein channel mimetic pumps"

#### Professor Blanca Lapizco-Encinas, RIT

"Novel strategies for particle manipulation with dielectrophoresis"

#### James McGrath, Univ. of Rochester

"Diffusion, Convection, Fouling and Sieving: How conventional transport concepts change when membranes are super thin"

#### Vincent Tabard-Cossa, Univ. of Ottawa

"Nanopores and Nanomembranes for Biomedical Applications"

# **Summer Picnic 2016**

























### **REU Program 2016**

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 Marguerite Weston. This summer (2016) 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 2016 REU Students (left to right, front to back):

1st Row: John Medina, Youngseon Park, Hannah Putman, Jose Luis Alvarez-Hernandez, Aubriana Perez, Merjema Purak.

2nd Row: Brandon Davis, Bailey Bowers, Sebastián Reyes De La Lanza, Lujain Felemban, Ana Capati, Hayden Carder.

3rd Row: Fulei Peng, Zach Kaye, Brandon Melenbacher, John Passanisi, Maria Alejandra Castellanos, Brittany Abraham, Yashika Sharma, Christine Burton.

4th Row: Henry (Jack) Gumina, Michael Gannon, Ilan Goldberg, Claire Dickerson, Tanya Townsend.

5th Row: Mitchell Miller, Alexander Strand, Marco Lopez, Paul Wrona, Yifei Liang, Alasdair Keith, Alex Callahan.

### International Student Research Program

In 2015 the Department inaugurated a Summer Research Fellowship Program (i-REU) designed to provide outstanding international undergraduates in Chemistry from all over the world the opportunity to conduct first class summer research at the University of Rochester. In this 2016 version the Department invited six very talented students coming from very different parts of the world (Cuba, Colombia, India, Korea, Mexico and United Kingdom) 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 chemistry department for 8-10 weeks. The experience for both the students and their hosts was terrific, and we look forward to watching these students become future scientific leaders.



2016 International Summer Students with mentors and faculty advisors

Bottom Row, left ro right: Reshmi Dani (Indian Inst. of Technology Guwahati–India, Physical Chemistry), Sebastián Reyes De La Lanza (U. Autónoma de Querétaro–Mexico, Physical Chemistry), Danielle Raymond (UR, Nilsson Group), Jennifer Urban (UR, Nilsson Group), Maria Alejandra Castellanos (U. Icesi–Colombia, Physical Chemistry), Youngseon Park (Seoul National U.–South Korea, Organic Chemistry), José Luis Alvarez-Hernández (Higher Inst. of Tech. and Applied Sciences–Cuba, Inorganic Chemistry);

Center row, left to right: Zhi Li (UR, Franco Group), Prof. Ellen Matson (UR, Physical Chemistry), Rachel Carey (UR, Franco Group), Brittney Patel (UR, Matson Group), Antonio Garzón (UR, Huo Group), Leah Frenette (UR, Krauss Group);

Top row, left to right: Prof. Ignacio Franco (UR, Physical Chemistry), Saikat Chakraborty (UR, Bren Group), Prof. David McCamant (UR, Physical Chemistry), Prof. Todd Krauss (UR, Physical Chemistry), Alasdair Keith (Heriot-Watt U.–United Kingdom, Physical Chemistry), Prof. Bradley Nilsson (UR, Organic Chemistry);

Not pictured: Professors Kara Bren (UR, Inorganic Chemistry) and Frank Huo (UR, Physical Chemistry).

# Pie in the Eye

Professors David McCamant, Josh Goodman, and Ben Hafensteiner all agreed to participate in the 2016 "Pie in the Eye" event held by the UR Student Organization (URSO) to support NY Special Olympics.

Special Olympics has held this event for the past three years in March, in which University of Rochester Faculty, Athletics, and Student Leaders sit in chairs and endure a "pie in the eye" in return for a small donation.







### **Grad Student Welcome Party**

On August 26th, 2016, the Chemistry Department finished up graduate 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!











### **Chemistry Welcomes 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

Kathryn (Katie) Knowles joined the Chemistry faculty in July 2016. Katie earned a B.S. in chemistry and a B.A. in mathematics from the University of Rochester in 2008. She then moved west to Chicago where she began graduate work in chemistry at Northwestern University under the guidance of Emily A. Weiss. Katie's Ph.D. work elucidated the influence of surface chemistry on the dynamics of photogenerated charge carriers in colloidal semiconductor nanocrystals, in particular, how surface ligands affect the ability of colloidal quantum dots to participate in photoinduced charge transfer reactions with small molecules. After earning her Ph.D. in 2013, Katie migrated further west to Seattle to start a postdoc position at the University of Washington with Daniel R. Gamelin. Her postdoctoral work explored the photophysics of luminescent semiconductor nanocrystals containing copper and their potential applications as phosphors in luminescent solar concentrators. Katie's graduate work and postdoctoral research were both supported by the U.S. Department of Energy through a DOE Office of Science graduate research fellowship and a DOE Energy Efficiency and Renewable Energy Postdoctoral Research Award, respectively.

Katie is thrilled to be returning home to Rochester to begin her independent academic career, and looks forward to developing a robust, world-class research program. She is excited to contribute to the education of undergraduate and graduate chemistry students at the University of Rochester, and began by teaching a graduate level course in Spectroscopy and Kinetics (CHM 458) in the Fall of 2016.

### **Selected Publications:**

Luminescent Colloidal Semiconductor Nanocrystals Containing Copper: Synthesis, Photophysics, and Applications. Invited Review. K.E. Knowles; K.H. Hartstein; T.B. Kilburn; A. Marchioro; H.D. Nelson; P.J. Whitham; D.R. Gamelin; *Chem. Rev.*, **2016**, *116*, 10820-10851.

Singlet-Triplet Splittings in the Luminescent Excited States of Colloidal Cu<sup>+</sup>:CdSe, Cu<sup>+</sup>:InP, and CuInS<sub>2</sub> Nanocrystals: Charge-Transfer Configurations and Self-Trapped Excitons. K. E. Knowles; H. D. Nelson; T. B. Kilburn; D. R. Gamelin, *J. Am. Chem. Soc.*, **2015**, *137*, 13138-13147.

Bright CuInS<sub>2</sub>/CdS Nanocrystal Phosphors for High-Gain Full-Spectrum Luminescent Solar Concentrators. K. E. Knowles; T. B. Kilburn; D. G. Alzate; S. McDowall; D. R. Gamelin, *Chem. Commun.*, **2015**, *51*, 9129-9132.

Electron Transfer as a Probe of the Permeability of Organic Monolayers on the Surfaces of Colloidal PbS Quantum Dots. K. E. Knowles; M. Tagliazucchi; M. Malicki; N. K. Swenson; E. A. Weiss, *J. Phys. Chem. C*, **2013**, *117*, 15849-15857.

Exciton Dissociation within Quantum Dot-Organic Complexes: Mechanisms, Use as a Probe of Interfacial Structure, and Applications. K. E. Knowles; M. D. Peterson; M. R. McPhail; E. A. Weiss, *J. Phys. Chem. C*, **2013**, *117*, 10229-10243.

Dual-Timescale Photoinduced Electron Transfer from PbS Quantum Dots to a Molecular Acceptor. K. E. Knowles; M. Malicki; E. A. Weiss, J. Am. Chem. Soc., **2012**, 134, 12470-12473.

# **Faculty News**

### Robert K. Boeckman, Jr.

Marshall D. Gates, Jr. Professor of Chemistry

### Ph.D. 1971, Brandeis University



### **RESEARCH INTERESTS**

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

#### CONTACT

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During the 2015-2016 academic year **ROBERT K. BOECKMAN, JR.** continued full time teaching and research, as well as his duties as associate editor of the *Journal of Organic Chemistry* and 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 aza-[3,3]-sigmatropic rearrangement methodology has been developed, which has now been published, and attention is now focused on application of this chemistry to the antitumor Manzamine class alkaloid Nakadomarin A. Work is continuing toward an asymmetric variant



The Boeckman Group

of a shelf-stable chromium(III) complex that serves as a precatalyst for Nozaki-Hiyama and Takai type chromium-mediated allylations of aldehydes and for a wide variety of chromium(II) mediated reactions, and also on asymmetric vinylogous Mukaiyama aldol reactions catalyzed by chiral oxazaborolidines. 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 toward asymmetric oxidation of aldehydes and other applications. Collaborations continue with DR. DAMIAN KRYSAN of the Department of Pediatrics(URMC), whose goals are 1) the identification of the biological target(s) of a novel series of small molecules which mimic the effects of caloric restriction on lifespan in yeast and in small mammals, and 2) the development of inhibitors showing specificity for fungal enzymes for use in antifungal therapy against invasive fungal infections of newborns and young infants. Exciting new collaborations between my group, DR. HALEBETINO (PH.D. '84) (Research Professor in Chemistry), and DRS. BRENDAN BOYCE and LIANPING XING of the URMC Department of Pathology and Laboratory Medicine have been established which 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.

HUI WANG (PH.D.'15) returned to China after completing a postdoctoral appointment with **ROBERT DEVITA (PH.D.'89)** at Mt. Sinai Medical School where he is employed at Novartis China in NATHAN E. GENUNG (PH.D.'10) Changshu. recently moved to Biogen Inc. in Boston as a Scientist JING ZHANG (PH.D.'01) recently joined Warp II. Drive Bio in Boston as Director of Chemistry. KYLE F. BIEGASIEWICZ (PH.D.'16) defended his thesis on FK-506 in October 2016, and moved to Princeton as a postdoctoral associate with Todd Hyster and to join his fiancée, Dr. Laura Ackerman (Weix group), who is also a postdoctoral fellow at Princeton in the group of Abigail Doyle. **DOUG TUSCH**, who is planning to defend his thesis early in 2017, is working on the Apoptolidin project with the assistance of fifth year student LIFENG XIAO and fourth year student KYLE Lifeng Xiao and postdoctoral associate RUGG. VENKATESAN SRINIVASAN (PH.D.'09) have been carrying out the preparation of bone-targeted drug conjugates, and promising leads have been identified for treatment of bone resorption accompanying rheumatoid arthritis therapy, and multiple myeloma in collaboration with Dr. Hal Ebetino of Chemistry, and Drs. Brendan Boyce and Lianping Xing from the URMC. Kyle Rugg is also working on a more refined route to Nakadomarin A. Second year graduate student **JUSTIN NIZIOL** is carrying on the synthesis of FK-506, picking up where Kyle Biegasiewicz left Part-time scientist DR. DENNIS SAVAGE, off. retired from Kodak, continues his work in the group on several projects with the Krysan group (Pediatrics URMC).



At the 2016 Graduate Student Orientation Poster Session

### Kara L. Bren

Professor of Chemistry

### Ph.D. 1996, California Institute of Technology



### **RESEARCH INTERESTS**

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

### CONTACT

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The **KARA BREN** group has had a productive and exciting year. Much of the group's efforts have been directed toward engineering metalloprotein and metallopeptide catalysts for small molecule activation. A major motivation is the development of new approaches to storing solar energy. The group also continued its work on magnetic resonance of metalloporphyrins, with a goal of developing high-performance magnetic resonance imaging (MRI) contrast agents with low toxicity.

The group was happy to welcome two new firstyear graduate students this year, **JENNIFER LE** and **SOMJIT BHAR**. Jen is working on engineering proteins into artificial hydrogenases, and Somjit is preparing novel metallopeptide catalysts for hydrogen evolution. Second-year graduate student **YIXING GUO** has made strong progress on developing metallopeptide catalysts for both proton and nitrite reduction. Third-

year graduate student SAIKAT CHAKRABORTY has been busy demonstrating the conversion of light to chemical energy in his focus on photocatalytic hydrogen production by biological catalysts. Fifth-year student **REBECCA SMITH** is wrapping up her work on manganese porphyrin MRI contrast agents and preparing to start teaching at Rochester Prep Charter School. Also completing her fifth year and her thesis work is BANU KANDEMIR, who has accepted a postdoctoral position with Prof. Jillian Dempsey at the University of North Carolina starting Fall '16. Postdoc PETER LAMBERG has brought the group in new directions with his development of a novel, easily fabricated bioelectrode that facilitates the storage and use of energy harvested from the metabolic processes of microorganisms. The group enjoyed working with our senior thesis students GIBRAN MANGUI (B.S. '16) and MARISSA GUERIN (B.S. '16). Gibran will be attending B.U. to pursue a Master's degree and plans



Kara Bren, Banu Kandemir, and Rebecca Smith next to the photochemistry apparatus used for photochemical hydrogen generation.
to apply to dental school. Marissa, who also earned a degree in film studies, returned home to Los Angeles to pursue opportunities related to science communication. The group also appreciated the close collaboration with DR. SANELA LAMPA-PASTIRK of the Krauss group, who is starting a tenure-track position at Nazareth College in Fall 2016, and we wish Sanela all the best in her new adventure. We were lucky to host two talented visiting Ph.D. students. INGVILD GUDIM from the University of Oslo worked on studies of electron transfer processes in microorganisms, and VINCENZO **FIRPO** from the University of Naples is studying fully synthetic metalloprotein catalysts. Finally, in the summer of 2016 the group welcomed two very talented summer researchers. Undergraduate CLAIRE DICKERSON (UR) worked with Yixing on metallopeptide catalyst development as part of the REU program, and JOSÉ LUIS ALVAREZ-HERNÁNDEZ (B.S. '15, Higher Institute of Applied Sciences and Technologies, Havana, Cuba) collaborated with Saikat on developing new approaches to photocatalytic hydrogen production sponsored by the Department's International REU Program.

Kara continued her role as Director of the Biological Chemistry Cluster, organizing the annual retreat and submitting a training grant application along with Co-PIs Rudi Fasan and Dan Weix (fingers crossed!) She also remains involved in the Society for Biological Inorganic Chemistry as a Council member on the boards for Accounts of Chemical Research and Comments on Inorganic Chemistry. Kara also is continuing her work as Associate Editor for the Journal of the American Chemical Society. She is very happy to work with VALERIE DRAKE as their office handles hundreds of manuscripts per year. Work involved a lot of travel again this year. A major highlight was celebrating Harry Gray's 80th birthday in Pasadena CA. Other highlights of Kara's seminar visits included Korea (Busan, Ulsan and Seoul), Beijing, Honolulu, Girona, and Prague.



The Bren Group

### Joseph P. Dinnocenzo

Professor of Chemistry



#### **RESEARCH INTERESTS**

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

CONTACT

jpd@chem.rochester.edu

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

Graduate student **ADAM FEINBERG** is nearing completion of his Ph.D. studies. As part of his Ph.D. work, Adam used nanosecond transient absorption spectroscopy to provide direct experimental evidence that alkoxyl radicals can react with pyridine bases to give pyridinyl radicals. As far as we are aware, these are the first examples of alkoxyl radicals acting as hydrogen atom donors in their reactions with a closed shell molecule. In addition, Adam is also working on the fragmentation chemistry aryltrialkyl Group 14 cation radicals. Adam has discovered that like aryltrimethylstannane cation radicals (previously investigated in the group by PULUO (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 provide important insight into the mechanism of these unusual reactions. Second-year graduate student **ANALUZ MARK** is currently working to extend the work started by Adam and Pu on novel fragmentation reactions of Group 14 cation radicals.

Joe also enjoys working in the lab on a fairly regular basis. He and colleagues **DR. SAMIR FARID** and **DR. RALPH YOUNG** are currently working on understanding several types of novel exciplex intermediates.

This summer the group had the pleasure of hosting **PROF. N. K. SULEMAN** and two of his undergraduate students (**AUBRIANA PEREZ** and **ANA CAPATI**) from the University of Guam for a summer research experience. It was delightful to have all three of them working in the lab with us and we look forward to hopefully continuing collaborative work with "NK" in future.

Over the past year the group added a femtosecond, tunable titanium:sapphire laser, a pulse selector capable of repetition rates up to 40 MHz, and a computercontrolled harmonic generator to their existing time-correlated single photon counting (TCSPC) apparatus. The new equipment provides a state-of-theart TCSPC system capable of excitation from the deep UV through the visible. This equipment will be used to study the dynamics of short-lived exciplexes.





Aubriana Perez and Ana Capati at the 2016 REU poster session

Joe and Bill Saunders

### **Richard Eisenberg**

Professor of Chemistry / Research Professor



#### **RESEARCH INTERESTS**

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

### **CONTACT** eisenberg@chem.rochester.edu

While **RICH EISENBERG** continues to be active in solar energy conversion and inorganic photochemistry, the past year witnessed the transition of his laboratory to a smaller footprint with fewer people. Rich's research continues to be collaborative, serving as co-Principal Investigator on two grants, one from DOE with KARA BREN as PI and TODD KRAUSS as the other co-PI, and the second, a just-funded award 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 the energystoring reaction of water splitting into  $H_2 + \frac{1}{2}O_2$  for solar energy conversion. Rich's group now contains two postdocs, with the possibility of an undergrad or two working in the lab. The first postdoc is **HONGJIN LV** who received his Ph.D. degree from Emory University and the second is **GUOCAN LI** who obtained his Ph.D. from Florida State University and just finished postdoctoral work at the University of North Carolina.

The publications of the past year document continued progress in Rich's focus on solar hydrogen and include efforts to make more effective light absorbers by either coupling strongly absorbing organic dyes to charge-transfer metal complex chromophores for enhancement of photoinduced electron transfer or stabilized quantum dots with different surface binding agents, and the first studies within the group on new photocathodes in order to eliminate the need for sacrificial electron donors in light-driven  $H_2$  generation.

Chemistry-related travels this past year included two named lectureships. The first, in late March, was at Washington University in St. Louis for the Marcus Memorial Lectures in which the speaker is chosen and hosted by graduate students; such occasions are always stimulating and enjoyable. The second was at Duke University for the inaugural Edinborough Instruments Lecture. The talk was presented in late April after





Rich and Marcia in New Zealand

having been cancelled in January due to an impending snow storm, a hazard of winter travel that Rich knows only too well. The trip to North Carolina also gave Rich and Marcia a chance to visit with good friends Maurice and Mary Hughes Brookhart, as well as some of the UNC faculty. In other chemistry travels, Rich attended meetings of the Board of Chemical Sciences in Woods Hole, MA and in Washington, DC, the DOE Conference on Solar Photochemistry and the annual retreat of the NSF-CCI on Solar Fuels directed by Harry Gray. Finally, and most important personally, Rich attended the special celebration for Harry Gray's 80th birthday at Caltech in November, in which he gave the after-dinner talk and led all in attendance in singing a Gray-modified "I Wanna Be a Producer". Rich also continues 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 travels that included a trip to the Canadian Rockies in August 2015, and Alaska in June 2016. Both offered some stunning scenery with ample evidence of glacial recession. It is symptomatic of global climate change and warming that must be addressed in our lifetimes. The latter of the two trips (Alaska) was part of a celebration of Rich and Marcia's 50th anniversary which will continue with a family gathering in NYC in October. And of course, there were trips to Washington, DC to see the granddaughters, as well as a family vacation in Turks and Caicos in February, the seventh time this biennial event has been held. Whether it is personal or scientific, Rich is a great believer in family and the ties that bind. Plans are being set for an eventful 2016-'17, as well as for Marcia and Rich's annual snow-bird migration to Sarasota, FL.

### **Samir Farid**

Research Professor



#### **RESEARCH INTERESTS**

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

**CONTACT** farid@chem.rochester.edu

**SAMIR FARID'S** research continues to be on photochemistry and the photophysics of electron transfer processes, in collaboration with Joe Dinnocenzo and Ralph Young. Our previous work on the effect of strong mixing on exciplex emissions and the role of varying degrees of charge transfer character was extended to the effect of solvent polarity on the degree of stabilization of the ion pair. Surprisingly, small changes in the structure of the donor or the acceptor have profound effect on the degree of stabilization of ion pairs. In low polarity solvents radical ion pairs ( $A^-D^+$ ) of equal redox energies are more stabilized when the acceptor is harder to reduce (more negative reduction potential) or the donor is harder to oxidize (more positive oxidation potential). That difference decreases with increasing solvent polarity and is absent in highly polar media – as the solvent stabilization becomes more important than the coulombic attraction.

Ph.D. 1967, Göttingen University

### **James M. Farrar**

Professor of Chemistry



#### **RESEARCH INTERESTS**

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

**CONTACT** farrar@chem.rochester.edu

Imaging ion-molecule reactions continues as the theme for **JIM FARRAR** and his research group. This year, we published a study of carbon cations condensing with allyl radicals, achieving an important milestone in our studies of ion-radical chemistry. Of course, 'milestone' for us means the paper has been downloaded three times. This year has also begun a time of transition for Jim's group. With the departure of postdoctoral fellow **DR. LINSEN PEI** for a position in the atmospheric chemistry group of Professor Lei Zhu at the Wadsworth Institute in Albany, Jim is taking the first steps in moving his crossed beam imaging instrument to Perugia, Italy, where Professor Stefano Falcinelli will employ it to study collisional ionization. Jim hope to make frequent trips to Italy to work with Stefano and his students. We have also continued our forty-year long collaboration with the Molecular Beam group in Perugia as Jim traveled to the "Elletre" synchrotron light source in Trieste for a series of experiments on multiply-charged molecular cations. Unfortunately, the earthquakes in Amatrice and Norcia caused this year's experimental run in November to be postponed.

After several years of teaching quantum chemistry to juniors and seniors during the Fall semester, Jim has switched his emphasis to teaching a one-semester course in general chemistry for engineers. Most of Jim's teaching career has been devoted to general chemistry, and although the work largely goes unnoticed, Jim believes that effective teaching of freshmen is an important activity. Even though today's freshmen expect to be taught differently than they were in the 1970s, the best students today are just as talented and stimulating as they were then. They just look younger! In addition to developing that new course, Jim also taught chemical thermodynamics, the second semester of physical chemistry, for the first time in nearly 30 years! He was quite busy preparing these two "new" courses. Happily, the most recent version of this course was better taught and received than it was 30 years ago.

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 a baby boy, Milo Martin, born November 30, 2016 to Mariana and Andy in Amherst.



**Rudi Fasan** Associate Professor of Chemistry



#### **RESEARCH INTERESTS**

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

**CONTACT** rfasan@ur.rochester.edu

PROF. RUDI FASAN and his group continue their research efforts toward the design and application of metalloprotein catalysts for synthetic applications and the investigation of new methodologies for the synthesis and evolution of macrocyclic peptide inhibitors of protein-protein interactions. Over the past year, the group has continued to expand the reaction scope of heme-containing proteins, specifically cytochrome P450s and myoglobins, to include synthetically valuable transformations that have so far remained restricted to the realm of transition metal catalysis. A team consisting of DR. SIMONE GIOVANI, former postdoc DR. RITESH SINGH, and third year graduate student HANAN **ALWASEEM** demonstrated that engineered myoglobins can efficiently catalyze the oxidative deamination of benzyl azides to yield aryl aldehydes (Chem. Sci. 2015). The same team subsequently discovered that P450 enzymes exhibit even higher reactivity in the context of this transformation, broadening its utility for the synthesis of electron-deficient ketones (ChemCatChem, 2016). ). After a very productive year as a member of the Fasan lab, Simone returned to Italy to take a senior scientist position at the biotech company BiosYnth. In another project, DR. VIKAS TYAGI (FLW, '16) demonstrated a first example of a biocatalytic Wittigtype aldehyde olefination reaction using engineered myoglobins as catalysts (Angew. Chem. Int. Ed., 2016). This transformation was applied to the olefination of a broad range of arylaldehyde substrates with excellent E-selectivity and catalytic efficiency, an accomplishment that was highlighted in Synlett and other journals. Based on previous mechanistic studies on myoglobin-catalyzed carbene S-H insertion, Vikas and other members of the lab were able to further expand the reaction scope of these hemoproteins for catalyzing asymmetric Doyle-Kirmse reactions (Angew. Chem. Int. Ed., 2016). At the end of the summer, the lab bid a fond farewell to Vikas who moved to a new position within the Centre

for Integrative Chemical Biology and Drug Discovery at the University of North Carolina at Chapel Hill. Using chemoenzymatic C-H functionalization, he and Hanan have successfully prepared novel analogs of the natural product parthenolide with improved antileukemic properties. This work, which was conducted in collaboration with the Jordan group at the University of Colorado, was described in a publication in Bioorg. Med. Chem.. Earlier this year, Hanan passed her candidacy exam, thus completing an important milestone toward her Ph.D. degree. In another exciting project, postdoctoral fellows DR. GOPEEKRISHNAN SREENILAYAM and DR. PRIYANKA BAJAJ were able to design efficient myoglobin-based cyclopropanation catalysts with stereodivergent selectivity. These new biocatalysts could be applied to enable the gram scale synthesis of various cyclopropane-containing drugs with excellent diastereo- and enantioselectivity. This work recently appeared in Angewandte Chemie as a 'hot paper'. The team working on metalloenzymes was joined this past year by new enthusiastic members of the group. These include first year graduate students ANTONIO TINOCO and ERIC MOORE as well as VIKTORIA STECK, who joined our graduate program after participating to our international REU program. This past year the group had also the pleasure to host MICHELE CROTTI, a visiting graduate student from the University of Milan who spent six months in lab to learn more about protein engineering and cytochrome P450 enzymes.

Important progress was also reported by group members engaged in our macrocycle projects. Using peptide cyclization methodologies recently implemented by the lab, third year graduate student **ANDREW OWENS** has recently succeeded in developing macrocyclic peptide inhibitors of the Hedgehog pathway, a key signaling pathway implicated in various types of cancer. Similarly, postdocs **DR. PHUONG THUC NGUYEN** and **DR. IVAN DE PAOLA** have made important steps forward in the design and optimization of cyclopeptide inhibitors of other cancer relevant protein-protein interactions. Ivan joined the group in the fall after receiving a Ph.D. and training in peptide chemistry from the University of Naples and the Italian National Center for Research (CNR) in Naples, Italy. During this past year, the group has continued to develop new methodologies for synthesis of macrocyclic peptides from ribosomal precursors (*Org. Biomol. Chem.*, 2016; *Meth. Mol. Biol.*, 2016).

In addition to the people mentioned earlier, the group has bid farewell to a number of talented undergraduate students who have graduated in May after conducting research in the Fasan laboratory. Our best wishes for a bright future and career go to CHRISTINE ZIEGLER (B.S. '16), who joined the biochemistry graduate program at the University of Michigan at Ann Arbor, GARRICK CENTOLA (B.S. '16), who joined the medicinal chemistry graduate program at the University of Maryland, KATHERINE GRASSO (B.S. '16), who will pursue a Ph.D. degree in chemistry at Boston College, and AMY (YI-WEN) LIU (B.S. CHEM. ENG. '16), who will start graduate school at Cornell University. The research accomplishments of our graduate and undergraduate students have been recognized by a series of college-wide awards, which

include a Hooker Fellowship to Andrew Owens, the Aynab Amin-Salem Memorial Prize to Christine Ziegler, and the Catherine Block Memorial Prize to **LAUREN BOLZ (B.S. '17)**. Congratulations also go to **RACHEL BONN** and **GARRICK CENTOLA** for being selected to present their research at the 2016 National Conference for Undergraduate Research (NCUR) in Asheville, NC.

Rudi and his students have also celebrated a new influx of funds to support their research. Earlier this year, the lab was awarded a three-year grant from the National Science Foundation to investigate P450-catalyzed C-H amination reactions and received seed money from UR Ventures (Technology Development Fund) to support a collaborative project with the Maquat lab at the URMC. In addition, the group was granted a University Research Award to support a cross-departmental project with Danielle Benoit (BME) and Benjamin Frisch (Medicine) aimed at exploring an innovative strategy for tissue targeted delivery of antileukemic compounds. External recognition of the lab's contributions has also translated into a busy traveling schedule for Rudi, who was invited to share the results of this group at several institutions and conferences across the US and abroad. During this past year, Rudi, Francesca, Penelope (4.5 year old), and Matteo (3 year old), have moved to a new house near Highland Park and they all enjoy the serene and friendly atmosphere of their new neighborhood.



### Ignacio Franco

Assistant Professor of Chemistry



#### **RESEARCH INTERESTS**

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

**CONTACT** franco@chem.rochester.edu

The **FRANCO** group is 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 three years in Rochester we have been building up the capabilities to investigate the general problem of how to control electrons using lasers, and the problem of how to develop novel multidimensional single-molecule spectroscopies in the context of molecular junctions. This year, our work on laser control was recognized by the NSF through its CAREER award. At the University level, the interdisciplinary aspects of our research have led to a joint appointment for Ignacio in the Department of Physics.

Our group of "Molecular Tortures" has seen several exciting additions in the last year. In September, **DR. BING GU** joined our group as a postdoctoral fellow after completing his Ph.D. at the University of South Carolina under the supervision of Professor Sophya V. Garashchuk. We are very excited to have Bing among our ranks as he adds tremendous expertise on quantum dynamics and talent into our team. Also, in January, two terrific Ph.D. students joined our group:



Front row: Bing Gu, Arnab Kar, Shi Li, Wenxiang Hu. Back row: Ignacio Franco, Rachel Carey, Antonio Garzon, Leopoldo Mejia.

**ANTONIO GARZÓN** from Colombia (Chemistry) and **WENXIANG HU** from China (Material Science). Antonio and Wenxiang are currently investigating the fundamental limits in the laser control of electrons. In addition, **LEOPOLDO MEJÍA**, also from Colombia, has now started his Ph.D. in the Department after spending last summer doing research in our group as part of our prestigious International Summer Research Fellowship Program. As part of that program, this summer we had the fortune of hosting **RESHMI DANI** from IIT Guwahati who analyzed single-molecule FRET data from the Krauss lab using Hidden Markov Models.

We have also seen several departures in the past year. In February, postdoctoral fellow **DR. LIPING CHEN** and visiting scientist **DR. LINJUN WANG** returned to China, where Linjun has taken a faculty position at Zhejiang University in Hangzhou. Also, in September, postdoctoral fellow **DR. ARNAB KAR** transitioned into a Research Associate position in the Laboratory for Laser Energetics here in Rochester. Our very best wishes to Liping, Linjun and Arnab in their new positions. We look forward to continued collaboration with them and watching them progress scientifically.

The group has been very active in giving talks and presentations worldwide. This past year, Ignacio was invited to give Departmental seminars at Los Alamos National Lab, Binghamton U., the Max Planck Institute for the Structure and Dynamics of Matter in Hamburg, Notre Dame and U. Copenhagen. He was also an invited speaker in Pacifichem (Honolulu, Hawaii), "Photodynamics" (Mendoza, Argentina), "ACS March Meeting" (San Diego), "Charge, Heat and Energy Transport in Molecular Junctions" (Copenhagen), and "Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy" (Telluride). Ignacio also had contributed presentations at the Gordon Research Conference on Quantum Control and the one on Donor-Acceptor Interactions.

Our molecular torturers in training, **ZHI LI** and **RACHEL CAREY** have recently delivered their third year talks and are now moving on to the last stage of their doctoral research. They were both awarded a NSF scholarship to attend the meeting "Toward Reality in Modeling Molecular Electronics" in San Sebastián (Spain) and present their Ph.D. research. In addition, the Department gave Zhi a travel award to attend the Gordon Conference on Donor-Acceptor Interactions; both Zhi and Rachel presented posters at this meeting.

In addition to conducting research and writing grants, Ignacio was a member of the Graduate Recruiting and Graduate Studies Committee. Ignacio has also continued to lead and advance a new Departmental program designed to bring top international undergraduate students to participate in research during the summer in Rochester. Ignacio also taught graduate Quantum Mechanics (CHM 451) in the fall for the third time, and Statistical Mechanics (CHM 455) in the spring for the second time. In addition, we had the pleasure of hosting **PROF. HERSCHEL RABITZ** (Princeton) and **DR. RALPH ERNSTORFER** (Fritz Haber Institute) during the school year.

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



Huo and Franco groups at Seabreeze Amusement Park

### **Alison J. Frontier**

Professor of Chemistry



### **RESEARCH INTERESTS**

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

**CONTACT** frontier@chem.rochester.edu

Professor **ALISON FRONTIER'S** research program is devoted to 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. Most recently, **YU-WEN HUANG (PH.D. '16)**, continuing the work of **JOSHUA BROOKS (PH.D. '12)** and **STEVEN JACOB (PH.D. '12)**, discovered a new cyclization cascade that assembles complex bridged bicyclic ring systems in a single step, from simple dienyl diketone precursors.

This year, we welcome **SHUKREE ABDUL-RASHAD** (B.S. University of Buffalo) to the group. We congratulate **YU-WEN HUANG (PH.D. '16)** who successfully defended his doctoral thesis last year. Yu-Wen is pursuing postdoctoral studies with Professor John Wood at Baylor University.



The Frontier group

### Joshua L. Goodman

Professor of Chemistry

### Ph.D. 1984, Yale University

Ph.D. 2011, Boston 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

goodman@chem.rochester.edu

**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

#### **RESEARCH INTERESTS**

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

**CONTACT** huo@chem.rochester.edu

The first year of the **HUO** group has been very exciting and productive. We have our group office in Hutchison Hall 431 fully renovated and our brand new cluster "Action" up and running and producing new quantum dynamics results. Four Ph.D. students, **SUTIRTHA CHOWDHURY**, **XINYANG LI**, **ARKAJIT MANDAL**, and **JUAN SEBASTIAN SANDOVAL**, and two postdoctoral scholars, **DR. SHARMA YAMAJILA** and **DR. FARNAZ SHAKIB**, have now joined us and bring their diverse backgrounds and research expertise to our group.

Sharma obtained his Ph.D. from JNCASR, India. He is developing new quantum dynamics methods that interface with scalable semiempirical electronic structure methods to simulate photo-induced charge separation dynamics in organic photovoltaics. He is also actively collaborating with the Bren and Matson groups on exploring hydrogen evolution and nitrite reduction catalytic pathways. Recently he won the 2016 Peter Salamon award from Telluride Science Research Center. Farnaz received her Ph.D. from University of Alberta, Canada. She brings her expertise on developing mixed quantum-classical dynamics methods and the knowledge of proton-coupled electron transfer (PCET) reactions to our group. Currently, she is developing new dynamics methods that are capable of describing non-adiabatic electronic transitions and nuclear quantum effects to simulate photocatalytic reactions.



Sutirtha recently graduated from IIT Chennai, India with a M.S. degree in theoretical chemistry. Xinyang got his B.S in chemistry from Wuhan University, China. They are currently working as a team to develop new ab-initio path-integral methods to simulate chemical reactions dynamics in condensed phase. Recently, they both won the "Materials Computation Center travel awards" (NSF-sponsored). Arkajit graduated from Visva-Bharati University in India, and Juan received his degree from Universidad Icesi, Columbia. This year, we also had undergraduates MARIA CASTELLANOS (Universidad Icesi, Colombia) and RACHEL CLUNE ('18) in our group conducting summer research. Maria's work on singlet fission quantum dynamics reveals mechanisms to potentially enhance fission yield and some of her results are currently being considered for publication.

Frank taught Computational Chemistry (CHM 469) for the first time and conducted numerous "computational labs" for the students in the class. They also used theoretical methods and simulation techniques from

The Huo Group

class to explore the topics relevant to their own research. The Huo group members have traveled around the world this year. Frank gave talks at the APS meeting in Baltimore, Boston University, the Telluride Excitation and Charge transfer workshop, and the ACS National Meeting in Philadelphia. In addition, Frank also presented the poster for the whole group at the Electron Donor-Acceptor Interactions Gordon Conference in Newport, RI. Sharma attended the Summer School on Fundamental Science for Alternative Energy at Telluride. Farnaz presented a poster at the Penn Conference in Theoretical Chemistry (PCTC) at the University of Pennsylvania in Philadelphia in August 2016. Both Xinyang and Sutirtha attended the Path Integral Quantum Mechanics: Theory, Simulation and Application workshop at CECAM in Lausanne, Switzerland and learned about state-of-the-art theories and computational methods for path-integral dynamics.

Looking forward to the next year, we plan to keep our momentum on research productivity as well as teaching and service efforts.

### William D. Jones

Charles F. Houghton Professor of Chemistry



#### **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; electro-philic C-H activation and direct routes to aromatic amines.

**CONTACT** jones@chem.rochester.edu

The **JONES** group continues our work in organometallic chemistry and catalysis. We had a new scientist join the group this year, DR. NAVEEN KULKARNI, who will be working on our joint project with Tom Baker at U. Ottawa to convert ethanol to butanol. DR. SUMIT CHAKRABORTY moved on to a new position at Tennessee Eastman. DR. SARINA BELLOWS took a job with SiGNa Chemistry Inc. here in Rochester. Our visiting professor from Huaihai Institute of Technology, DR. RUI-BO XU, returned to China, but PROF. HENG ZHANG from Wuhan University came to work in our group for one year. We had 2 undergraduate REU students for the summer, and DR. FAZLUR **RAHMAN** from the Oklahoma School for Science and Mathematics returned to Rochester for a summer of research. (Fazlur was here in 1998 in our RET program.) Our research is examining the activation of C-H bonds in substituted hydrocarbons, C-S cleavage and functionalization reactions, 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 just filed a patent on this discovery. The group continues its role in the Center for Enabling New Technologies through Catalysis (CENTC), in which the group has collaborative research projects that are exploring new electrophilic C-H activation catalysts, new direct routes to aniline from benzene, and the above mentioned butanol process. Bill continues as Associate Editor for the Journal of the American Chemical Society for a thirteenth year, where he handled close to 500 manuscripts last year. He gave talks at SUNY Cortland, Ithaca College, the Universidad Nacional Autonomas de Mexico (UNAM), and King Abdullah University of Science and Technology (KAUST). He also spoke at Pacifichem in Honolulu, the ACS National meetings in Boston and San Diego, the 3rd International Symposium on C-H Activation in Montreal, and at the International Conference on Organometallic Chemistry, in Melbourne, Australia, July 17-22 2016, on "A new tandem route for conversion of ethanol to butanol." 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).

Our work in C-H activation is also continuing in a collaborative research effort in the Center for Enabling New Technologies through Catalysis (CENTC). This NSF-funded center includes researchers from a dozen universities participating in joint projects and using cyber-conferencing to discuss results. This mode of research is testing a new paradigm for conducting collaborative research and is beginning its tenth year of phase 2 funding (\$4M/yr). Our group has completed several collaborative projects with the Goldman group, the Mayer group, the Miller group, and the Cundari group through CENTC, and will continue with 4 projects this year.

Bill will serve on the International Advisory Board

Visit to KAUST, Saudi Arabia

for the ICOMC, ISCHA, and OM&Cat conferences. The group is supported by continuing funding from the Department of Energy, the National Science Foundation, and the NSF Center Enabling New Technologies through Catalysis.

Bill's grandson, Henry William Simson, born to his daughter Sarah and her husband Michael, is now 2 years old. Henry is thriving, and Heather and I are delighted to see him often since they live in Rochester near Sea Breeze. Our oldest daughter Elizabeth was married last summer to Josh Sweet, and they now have a house in Chili. Simon continues at iHeart Radio where he was recently promoted to Art Director.



Snorkeling with a few faculty in the Red Sea, near KAUST

## Todd D. Krauss

Professor of Chemistry



#### **RESEARCH INTERESTS**

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

**CONTACT** krauss@chem.rochester.edu

What happened in the **KRAUSS** group this past year? Some comings and goings, some travel, some papers in various stages, and some unsolved mysteries....

**DR. SANELA LAMPA-PASTIRK** left the group to take a position as an Assistant Professor of Chemistry at Nazareth College in Pittsford. When she is not buried in administrative paperwork she assures us that she will come around the lab from time to time helping with the ultrafast lasers or growing bacteria for solar fuels production. Congrats to Sanela on her new faculty position! KELLY SOWERS(PH.D.'16) and AMANDA PRESKE (PH.D.'16) both defended their theses this summer and went literally in two completely different directions for their post Ph.D. positions. Kelly went to the Netherlands for her postdoc to work with Celso de Mello-Donega at the Debye Institute for Nanomaterials Science at the University of Utrecht. She is very excited about a position with one of the top nanoparticle laboratories in Europe! Amanda decided to fully explore her artistic talents after graduation. She stayed in Rochester to work on developing her rapidly expanding business (Circuit Breaker Labs) where she sells her handmade circuit board jewlery. Amanda was recently featured with a front page article in the local newspaper Democrat and Chronicle Sunday Business section describing her unique art! (For those interested a sampling is here: https://www. etsy.com/shop/CircuitBreakerLabs) Congratulations to Kelly and Amanda and best wishes on your future careers!

**NICOLE M. B. COGAN** spent a lot of the past 2 years studying what we thought were single molecule color center defects in quartz. We were wrong, and good thing! In a remarkable discovery, Nicole found that toluene, poly(methyl methacrylate) and parafilm combine in as yet unknown ways to make a molecule with truly amazing photophysical properties including

the ability to emit "quantum light" continuously. Working closely with Alison Frontier's laboratory, we hope to identify the sturucture of the mysterious molecule shortly. **ZHENTAO HOU** is working on her first paper! She is reporting on some very interesting observations of the effect of small moleule reductants on the photoluminescence of carbon nanotubes. Zhentao found that depending on the surfactant used to solubilize the nanotubes, she can increase or decrease the photoluminescence substantially. Her work shows that the surfactants around nanotubes may not be as innocent as we thought with respect to influencing the photophysical properties of the nanotube.

This past summer "world traveler" LEAH FRENETTE added another continent to her resume. She was recruited to go to Japan to attend a conference related to alternative energy production. When not jetting around the globe, Leah is finishing up her paper on how the old ways of making quantum dots from the late 1980s are actually what is taking place in the reaction vessel upon breakdown of the "modern" chemical precursors. Watch out NOLA! AMANDA AMORI is going to present her exciting work on the intervalley scattering of the exciton in carbon nanotubes at the APS meeting in March of 2017 in New Orleans. I expect Amanda's talk will be as well received as the local beignets! Amanda is also working on some really hard measurements of trion photophysics in single nanotubes at low temperature that we hope to report on next year.

**ABBY FREYER** is trying to understand what happens when CdSe quantum dots are doped with silver ions. She has gotten some great data on the relationship between the photoluminesence and the average charge properties of the doped quantum dots using electrostatic force microscopy, which is extremely hard to pull off on the single particle level. Working with researchers at Cornell University, Abby hopes to use fancy electron microscopy techniques to locate the silver atoms in the CdSe lattice and thus complete the picture of what is going on in the doping process.

JENNIFER URBAN, our first joint Nilsson-Krauss student, is going skiing in Aspen in January! Also, at the same venue, she will be reporting at the single molecule biophysics conference about how she attaches amyloid Beta fragments onto CdSe quantum dots to create oligomer mimics and studies how they are internalized by neurons with super-resolution microscopy. The expectation is that the particles will behave as toxic amyloid Beta oligomers, and identifying where they are in the cell could help elucidate a mechanism for their toxicity. Finally, in a very difficult synthesis BECKAH **BURKE** has made CdTe/CdS/CdTe nanobarbells which she used in combination with small molecule metal catalysts to reduce protons to the clean burning fuel hydrogen. She is working on quantifying how much better the barbells are than traditional, spherical quantum dots and we are excited because preliminary results suggests the barbells work great!

During the summer the group hosted rising UR Chemistry graduate student **JORDAN ANDREWS** from St. John Fisher College, **BRANDONMEHLENBACHER** (younger brother of UR alum **RANDY MEHLENBACHER**) from SUNY Geneseo and **ALASDAIR KEITH** from Heriot-Watt University in Scotland. Jordan worked with Amanda Amori on isolating nanotubes of different chiral species. Brandon worked with Beckah on making nanobarbells of narrow diameter such that they absorb green and not red light with applications to solar fuels production. Alasdair worked with Leah on synthesizing highly fluorescent PbS and PbS/CdS quantum dots in very high concentrations for a quantum dot SPASER in collaboration with the Odom group at Northwestern.

Finally, **LISA CARLSON NOGAJ (PH.D.'09)** and **KATIE LEACH (PH.D.'09)** put together a facebook page for the Krauss group! We use it to stay in touch with current members and alums. <u>https://www.facebook.com/groups/kraussgroup/</u>



The Krauss group summer outing to the Red wings Game

### **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

During the past year **TOM KRUGH** continued his support of graduate and undergraduate education. During the spring and summer his main project involves organizing our NSF-supported Research Experience for Undergraduates (REU) program with the expert assistance of Marguerite Weston. This summer (2016) 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.



## Ellen Matson

Assistant Professor of Chemistry



#### **RESEARCH INTERESTS**

Probing cooperative reactivity between non-traditional ligand platforms and first-row transition metal centers, specifically their ability to facilitate chemical transformations of industrial, environmental and biological significance. Developing the chemistry of early to mid first row transition metals, specifically investigating their catalytic applications in an effort to develop orthogonal systems for complex organic transformations.

**CONTACT**: matson@chem.rochester.edu

What a year for the Matson Lab!!! We've gone from a group consisting of **ELLEN MATSON** and her husband **SCOTT** HICKS, to a team made up of a fabulous postdoctoral researcher, three all-star graduate students and some of the best undergraduate researchers that U of R has to offer (in Ellen's opinion). First to join the group, was our postdoctoral researcher, DR. FENG LI (Notre Dame, Ph.D.). Feng spent his graduate career investigating the synthesis of main group cluster complexes with Prof. Slavi Sevov. Soon after the beginning of the school year, LUJAIN FELEMBAN('17) and MERJEMA PURAK ('18) joined the team. Both undergraduate researchers have been central in helping Ellen get the lab up and running. In December, we welcomed our first class of graduate students, **RACHEL MEYER** (Hood College), BRITTNEY PETEL (U. Delaware) and LAUREN VANGELDER (U. Buffalo). These women took on the challenge of joining a brand new research program. This summer, our laboratory expanded with many summer researchers, including three rotating first-year graduate students and an international REU student. This fall,

our most recent addition, undergraduate MEGAN NGAI ('19), joined the Matson Group. Each new member of our lab this year expanded our research family and added lots of depth to our group's scientific ambitions. All of the group members have had an extremely busy year - working hard to get our chemistry off the ground! Some highlights from the first-year of the Matson Lab included moving into our beautiful renovated lab space (come by and check out our beautiful blue lab in HHB50!). We also had a couple of exciting "firsts" - most notably, we published our research group's first paper (DOI: 10.1021/acs.inorgchem.6b01349, great work Feng and Lauren!!). Ellen was selected to give a poster-talk on the group's research at the Inorganic Gordon Research Conference this summer, an exciting honor for a first-year faculty member! Diving back into the school year, we're looking forward to building upon our successes from the 2015-2016 school year and continuing to grow our group! Follow us on twitter (@MatsonLab) to stay up to date with the latest developments from the Matson Lab!



The Matson Group

### 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 photo-excited nucleic acids; Ultrafast energy and electron transfer processes relevant for solar energy systems.

#### CONTACT

mccamant@chem.rochester.edu



Prof. McCamant and graduate student, Joohyun Lee, developing new femtosecond spectroscopy

The **MCCAMANT** group is doing great this year, with a strong group of graduate and undergraduate students tackling the challenges of studying ultrafast photochemical dynamics. Postdoc DR. COLLINS NGANOU, now at Cape Breton University, completed his fascinating molecular dynamics study of thyminethymine dimers, which showed that the most recent DNA force fields are not quite right for single stranded DNA. ZAK PIONTKOWSKI (CHE B.S. '14) passed his qualifying exam with flying colors this summer and is charging ahead with joint experimental-theoretical studies of how dye-bridge torsional dynamics can affect electron transfer rates relevant to solar fuels production. MIKE MARK is pursuing femtosecond laser studies of a variety of organic dyes that are used for solar hydrogen production, though he took a break from that work to travel to Swaziland for four weeks in order to do chemistry outreach as part of the University's IGERT program for sustainable energy research. Mike has also built an outstanding CW Raman facility that will be used

by the entire department and visiting scientists and was funded by an NSF MRI grant to Profs. Neidig and McCamant. Mike and **JOOHYUN LEE** spearheaded the big repair that our femtosecond titanium-sapphire oscillator laser required this year, so now things are up and running and back on track. Joohyun Lee is working hard to finish his dissertation that probed the structural dynamics of the dGMP nucleoside after it absorbs ultraviolet light. In the fall of 2016, **ZHI WU**, a visiting student from Xiamen University, joined our team. Zhi is supported by a fellowship from the Chinese Scholarship Council to pursue solar hydrogen research in our lab through 2018.

This year we had the pleasure of working with a great group of undergrads. **AMANDA CARR (B.S.** '16) brought our group into the interesting world of infrared spectroscopy, developing an entire new class of experiments that we continue to pursue in the process, and will be pursuing graduate studies at Stony Brook

University. **SARAH PRISTASH (B.S. '16)** received the ACS award for Outstanding Achievement in Chemistry from the ACS's Rochester local section as well as the Carl Whiteman Award for undergraduate teaching. Sarah will be going to graduate school at the University of Washington this fall. **DYLAN BLEIER (B.A. '16)** did some of the first, and perhaps the last, molecular synthesis in our lab as he pursued a variety of studies of dye-sensitized semiconductor systems; Dylan will be attending the University of Wisconsin's graduate program next fall. **JESSICA FREEZE ('17)** did great

work with us throughout the year studying everything from CW Raman spectroscopy to computational studies of molecular vibrations. We're looking forward to her return this fall as she completes her senior research in our lab after spending this summer in an REU program in Minnesota. Lastly, **BAILEY BOWERS**, an REU student who is a rising senior at Wooster College in Ohio, worked with us this summer using infrared spectroscopy to study bridge and anchor groups attached to titanium dioxide.

### John S. Muenter

Professor Emeritus of Chemistry

### Ph.D. 1965, Stanford University



#### **RESEARCH INTERESTS**

Molecular spectroscopic studies of inter- and intramolecular interactions using molecular beam, microwave, and laser techniques.

#### **CONTACT** muenter@chem.rochester.edu

For **JOHN MUENTER**, the past year has progressed much like the past few years; busy with nonacademic interests: travel, family, classical music, etc. He still goes to 20 to 25 operas a year and volunteers for the Friends of Eastman Opera, an organization that benefits Eastman School voice and opera students. John's two grandchildren have gotten a year older, 6 and 3 now, and his daughter is enjoying being a tenured chemistry prof at Denison University in Granville, Ohio. Molecular spectroscopy is still important to him and he continues to spend one week every couple of months working at MIT with Bob Field's graduate students. A minor change in the basement of Hutchison has produced a major amount of work for John; he is finally leaving his old office, B36. He was the very first person to move into Hutchison in 1972 and it is amazing how much junk can accumulate in an 8' X 12' windowless office in 44 years. John was able to attend Bill Saunders' 90<sup>th</sup> birthday celebration in August 2016, and had a good time sharing stories with everyone at the event.



### **Michael Neidig**

Assistant Professor of Chemistry



#### **RESEARCH INTERESTS**

Physical-inorganic chemistry and catalysis: elucidation of structure and bonding in nonprecious 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 during their fifth year at Rochester. The group currently consists of seven Ph.D. students and one postdoctoral scholar, with JEFF SEARS (Georgia State) joining the group this past Fall. We were also excited to have FULEI PENG ('16) with us again last year. We had the pleasure of hosting several visiting international scholars throughout the year, including PROF. BERT KLEIN GEBBINK (U. of Utrecht) who spent a sabbatical in our group, DR. RUTH WEBSTER (Bath) and PETER NEATE, a Ph.D. student from the University of Edinburgh. The group once again hosted students from Monroe Community College and local high school students for summer research experiences. We had another highly successful research year, highlighted by a study elucidating a key iron species in cross-coupling with simple iron salts that had been a mystery for over 40 years.

We were excited to receive a Department of Energy Early

Career Award grant this year to expand our research into f-element chemistry - an exciting additional research direction for the group. Graduate students in the group were honored with several awards including a poster prize at the Inorganic Discussion Weekend meeting in Kingston, ON (TESSA BAKER) and a Hooker Fellowship (JARED KNEEBONE). Mike was constantly on the move this past spring as he embarked on a prolonged seminar tour highlighting the group's research accomplishments, including trips across the country as well as a two week tour of universities in the UK. More recently, Mike gave an invited talk at the ICCC conference in Brest, France. Lastly, Mike was honored to be appointed the Wilmot Assistant Professor of Chemistry this summer – an accomplishment attributed to the tremendous work of all the members of the group. Moving forward, we anticipate another exciting year of research in non-precious metal catalysis and f-element chemistry at Rochester.



### **Bradley L. Nilsson**

Associate Professor of Chemistry



#### **RESEARCH INTERESTS**

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

**CONTACT** nilsson@chem.rochester.edu

The **NILSSON** group has had an exciting year during 2015–2016. Graduate and undergraduate students are graduating, advancing, publishing, and experiencing significant life events. **JOHN DIMAIO (PH.D. '15)** defended his PhD thesis entitled "Functional Materials Composed of Supramolecular Fibrils". John completed his thesis after starting studies at the Law School at the University at Buffalo in the Fall of 2014. He's relieved to be a "single-discipline" student in law now that his Chemistry Ph.D. work is complete! John will complete his law degree in 2017 and has been offered a position at Hodgson Russ in Buffalo, NY in the area of intellectual property law. We're thrilled for his success and congratulate him for heroically keeping so many things afloat at once!

**ANNADA RAJBHANDARY (PH.D.'16)** also completed her Ph.D. studies this year. Her thesis, "Investigating the Relationship Between Structure and Self-Assembling Behavior of Fmoc-Protected Phenylalanine Derivatives", has resulted in one publication to date (*Biopolymers* **2016**, *106*, DOI: 10.1002/bip.22994) with several others currently under review. She was also married in February 2016! Following the completion of her studies in August 2016 she returned to her native Nepal with her husband, where she hopes to find an academic position.

### DANIELLE (RAYMOND) RIEGLE and JEN URBAN

have made significant advances in their research projects and have the final completion of their Ph.D. projects in sight. Danielle continues her study of 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. Danielle was married this summer to her fiancé, Clint Riegle. We congratulate her on her marriage as well! Jen, a member of both the Nilsson and Krauss groups (in collaboration with Handy Gelbard in the University of Rochester Medical Center), is bravely forging a path in a new research area for all of our groups, the application of quantum dots for super high resolution imaging of cellular processes. She is building microscope instrumentation, adapting analysis software, synthesizing peptides, and functionalizing quantum dots! She's a true renaissance woman and is a master of multitasking.

**JADE WELCH** made significant progress in her research this year. She was primary author on a paper detailing the use of cyclic peptides for the *in vivo* delivery of therapeutic oligonucleotides to the lung (*ACS Med. Chem. Lett.* **2016**, *7*, 584). We congratulate her on this important achievement! Her work is now focused on the mechanism of action for 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 was engaged to her fiancé, Blake Russell, in July 2015. We congratulate them both!

**PAUL RUBEO** recently progressed to Ph.D. candidacy in June of 2016 and is entering his third year in the Nilsson lab. He is excited to continue his work on low molecular weight amino acid-based gelators and in the development of novel fluorescent detectors of amyloid fibrils. His work is going well and we recently submitted his first manuscript for publication. He is also looking forward to continuing his work with the Horizons program and other education based service opportunities. In his personal life, we congratulate Paul on his engagement to his fiancé, Mikella. The two will be getting married in September of 2017.

The Nilsson group has been fortunate to work with a number of talented undergraduate researchers in the last year. **SAGAR PATEL (B.S.'16)** completed his senior thesis research in the Nilsson group in the last year, with a project focused on understanding the self-assembly

of hydrogel-forming peptides. Sagar is currently working and applying to medical schools for admission in 2017. ADRIAN ROSENBERG (B.A. '16), PAIGE PALMIERI (B.A.'16), and KELSEY TUTTLE (B.A.'16) also conducted undergraduate research projects during the last year and finished their undergraduate studies in the spring. Adrian is taking a gap year to travel in South America prior to applying to medical school, Paige has joined the graduate program in Food Science at the University of Wisconsin-Madison, and Kelsey (who also completed a degree in business as well as chemistry) is currently working in Wyoming and applying to medical schools. We're confident in their future success and congratulate them on completion of their studies. CHENGYENG LI, another University of Rochester undergraduate, also joined the Nilsson group during the last year. He has been working on the synthesis and analysis of self-assembling peptides towards the creation of novel biomaterials. JANSON HO has spent the last several years conducting research in the Nilsson group. In fall 2016, he presented his work from the Nilsson group and was selected for a presentation award at the AIChE Undergraduate Poster Competition in Salt Lake City, Utah. This summer, Janson worked in Baton Rouge as a Research and Technology intern at the specialty chemicals company Albemarle, conducting research on process development and optimization. Currently, he is having a wonderful time on his exchange abroad in chemical engineering at the Hong Kong University of Science and Technology for the fall term, but looks forward to returning in the spring.

BRITTANY MURPHY (SUNY GENESEO) and NATIONAL YOUNGSEON PARK (SEOUL UNIVERSITY, SOUTH KOREA) also conducted summer REU research in the Nilsson group during 2016. They were outstanding research students and made significant progress in their work in a short period of time. They were excellent additions to the group during their time at the University of Rochester. We have welcomed two new undergraduates into the research group this year, **PRESTON HOLLOPETER** and **MATT** WATROUS. Both are quickly learning and making strong contributions to our research efforts. We look forward to continuing to work together in the coming year.

**WATHSALA LIYANAGE (PH.D.'15)**, a recent graduate from the Nilsson group, and her husband, Sudath, recently welcomed their first child, Shenya, on March 19, 2016. She was 6 lbs, 14 ounces, and is happy and healthy. Mother and father are adapting to life as parents. We're thrilled for Wathsala and Sudath!

In addition to managing a busy research group, Brad has stayed busy 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). At home, Brad and Trista sent their oldest daughter, Emma, off to college this fall (Brigham Young University) and are coping with the realization that they are actually old enough to have a college student!



### Lewis J. Rothberg

Professor of Chemistry



#### **RESEARCH INTERESTS**

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

**CONTACT** rothberg@chem.rochester.edu

LEWIS ROTHBERG's group continues to research luminescent conjugated polymers relevant to organic light-emitting diode technology. Three students graduated with their doctoral degrees this year including MILLARD WYMAN (PH.D.'16) (delayed photoluminescence in ladder polymers), CHRIS FAVARO (PH.D.'16) (outcoupling of light from emissive devices using silver nanoparticles) and BEN MARTIN (PH.D.'16) (single polymer chain spectroscopy). Millard is now teaching Chemistry and Physics at St. John Fisher College while Chris and Ben have moved on to industrial positions (Chris at Kateeva and Ben at Sydor Instruments). Chris' thesis, done on work that was in collaboration with **PROF. CHING TANG**, evolved from a crude general idea into a beautifully documented, argued and written piece of science. Ben's work discovered surprising oxygen effects on polymer luminescence and stimulated new ideas and directions that resulted in a successful NSF proposal this year. In the meantime, RAJ CHAKABORTY has completed his lab work studying magnetic field effects on delayed luminescence and is now writing up his work for publication and preparing to graduate. He spent a summer working at an internship at Apple and learned a lot about life beyond graduate school.

Chemical engineering graduate student **CHEN ZHANG** has done fine spectroscopic work with senior scientists **AL MARCHETTI** and **RALPH YOUNG** to understand interfacial charging in model OLED structures. Obtaining research funding continues to be difficult, and Lewis is spending more time in the lab with the graduate students and excellent undergraduates **MATT CARBONE (B.S.'16)** (photothermal absorption of ultrathin polymer films) and **CHRIS MELNYCHUK (B.A.'16)** (plasmon stabilization of fluorophores). Chris is now helping Lewis to transition some of his research to do transient vibrational spectroscopy aligned with a broad, exciting collaborative initiative in the department to work on sunlight driven catalysis to make transportation fuels from abundant materials. Lewis hopes to contribute to this exciting and important new direction, having realized that solving our energy problems in an environmentally responsible way is among the most important challenges facing modern society.

Both Lewis and the students presented work at a variety of ACS and Materials Research Society meetings. Most memorable for Lewis was giving the plenary talk at the 11th meeting on Optical Probes of Conjugated Polymers in Hong Kong. Lewis has attended every one of the 11 meetings (since 1992) and is co-founder of the very successful series with Valy Vardeny at the University of Utah. It still remains a flagship meeting for spectroscopy of organics, a field that remains problem and technology rich even nearly 30 years after Ching Tang's seminal OLED work. Lewis has been blessed to see much of the science and technology evolve. The meeting was coupled with a memorable highlight of the year, sharing local sites and culture with friend and colleague Ching Tang, who is now on the faculty at a new institute at HKUST and a native of Hong Kong.



Dr. Ching Tang



Lewis taught the junior level statistical thermodynamics (CHM 252), a course that continues to fascinate. He continues to teach the advanced spectroscopy lab (CHM 232) with a lot of help from **RAY TENG (B.S. '83, M.S. '87, M.B.A. '01)** and a strong cadre of teaching assistants. Lewis plans to work with colleagues in Physical Chemistry to add more modern labs to the course and update the manuals over the next several years. In the fall, Lewis is excited to be teaching junior level quantum chemistry for the first time and looking forward to the rich understanding that preparing a course often brings.

Lewis remains director of the Materials Science program at the University, a Ph.D. and M.S. granting program that has now grown to nearly 50 students. The program is ably administered by **GINA EAGAN**. The faculty banded together for an internal brainstorming meeting with the intent of preparing a strong Materials Research Center proposal to the NSF. We are also introducing new pedagogical and team-building programs for the cadre of materials science students.

Diffinity Genomics, a small biotechnology company formed to commercialize technology developed in our lab by DR. HUIXIANG LI, struggled once again this year, but has nevertheless continued to sell products. Fortunately, the company's technology has attracted a buyer and has been purchased by Chiral Technologies, a much larger company capable of expanding sales and distribution. In part, this was possible since the patent on the UR owned molecular separations technology at Diffinity's core was issued in spring 2016. It is likely that Lewis will continue to consult with Chiral Technologies on R&D to underpin future products in the genomics space that exploit some of the ideas developed by Diffinity. Lewis enjoyed recounting his entrepreneurial experience at a local ACS meeting and for the students in the NSF-REU summer program, and remains grateful to the department and University for the flexibility enabling him to learn and grow in different ways.

On a more personal note, Lewis lost his beloved mother **PROF. ESTHER CONWELL** in November 2014,

also a departmental stalwart whose affiliation with UR Chemistry long predates Lewis' employment. The department kindly sponsored a moving memorial service in March 2015 at the UR Chapel. Esther was widely cherished in the scientific community and garnered many awards and accolades. She continued to do publishable research until she died at 92 with manuscripts under review and more in preparation.



Lewis was able to join Esther's friends and colleagues in the chemistry and physics community in June 2016 to celebrate her life and accomplishments with a special session in her honor that was held at the International Conference on Synthetic Metals (ICSM) in Guang Zhou China. One of her former postdocs, Dr. Ming-Wei Wu, gave a talk entitled "The Meaning of Life" at the memorial symposium in her honor. He told the story of how they met and how his relationship with Esther evolved from that of mentee to colleague and friend. She continues to be deeply missed by Lewis, his wife Shelby, and their children Charles and Vivian. The Esther M. Conwell Graduate Fellowship Fund was established by Lewis and Shelby to provide stipend support for advanced graduate students in Chemistry who show exceptional promise as researchers.



Dr. Ming Wei Wu and Esther Conwell in 1996 59

### Wolf-Udo Schröder

Professor of Chemistry

### Ph.D. 1971, University of Darmstadt, Germany



#### **RESEARCH INTERESTS**

Basic and applied nuclear science: dynamics of complex nuclear reactions at intermediate and high energies; dissipation, relaxation and other transport phenomena; nonequilibrium effects; thermodynamics of nuclear disintegration and transmutation; the equation of state of nuclear matter. Beyond the mean field: correlations and clusterization of nuclear matter. Light-ion reactions in a thermonuclear environment. Chemi-and physisorption of tritium in metals.

#### **CONTACT** schroeder@chem.rochester.edu

**W. UDO SCHRÖDER'S** Nuclear Science Research Group has continued research in radiochemistry, heavy-ion reaction dynamics, advanced detector development, as well as with the development of Laser Ion Acceleration for Nuclear Science. Three students **(ERIC HENRY, SHETH NYIBULE, and MATTHEW SHARPE)** have successfully defended their Ph.D. theses. All of them have found gainful employment; Eric at INTEL, Sheth at RIT, and Matt at LLE. Eric and Sheth had the opportunity to present their results at the Gordon Conference on Nuclear Chemistry in an invited talk or a poster presentation, and Matthew spoke at an international conference on Tritium and its applications. Udo gave a colloquium at Texas A&M University and lectured on the UR Campus on nuclear

### **Douglas H. Turner**

Professor of Chemistry

energy issues. As Scientific Editor, he has accepted, and almost completed, the task of putting together a book on *Nuclear Particle Correlations and Cluster Physics* for the World Science Publishing Co. The group's contribution to that book describes a stunning observation of a necklace-like disintegration pattern of an intermediate system produced in energetic heavy-ion reactions (Sheth's thesis work).

A number of new experiments were conducted with a group at LLE, using the OMEGA laser facility as an extremely bright neutron source. Work continued also on technical R&D with novel scintillator materials and on the detailed radio-chemical study of tritium migration through metals.

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

The Turner group continues to develop and apply methods for determining RNA folding and to apply those methods to targeting influenza A. **Jon Chen** (PH.D. '16) published a paper that extended the NMR Assisted Prediction of Secondary Structure (NAPSS) method first developed by **JIM HART (PH.D. '08, M.D. '10)**. The extension allows determination of the direction of a helix by considering chemical shifts in base pairs. Jon also published a chapter in a book, "RNA Structure Determination," edited by Doug and **DAVE MATHEWS (PH.D. '01, M.D. '03). SUSAN SCHROEDER (PH.D. '02)** contributed to the book a chapter on her computer program, Crumple, for rapidly finding all possible secondary structures for an RNA sequence. The book is a volume in the Methods in Molecular Biology series.

NMR and computational studies continue in the group with the research of graduate students,



**ANDY KAUFFMANN, KYLE BERGER,** and **JIANBO ZHAO**, along with longtime collaborator, **SCOTT KENNEDY**. Scott also contributed a chapter to the book mentioned above. In a University wide competition, Andy won a Hooker Fellowship.

The group continues to study influenza in collaboration with **Luis Martinez-Sobrido** in the Department of Microbiology and Immunology and with **Ryszard** and **Ela Kierzek** at the Institute of Bioorganic Chemistry in Poznan, Poland. **Ela Lenartowicz**, who is the first Ph.D. graduate from E. Kierzek's group, started as a postdoc in Rochester. She published her thesis research determining the secondary structure of an influenza genomic segment. This was followed with a paper showing that oligonucleotides targeting the structure can inhibit viral propagation in cell culture by up to 25fold. She also designed the cover of the issue of Nucleic Acid Therapeutics that included this paper.

In another approach to influenza, **TIAN JIANG (PH.D. '15)** used a thermodynamic approach, called ensemble defect, to design a minimal number of mutations (2) predicted to completely change a conserved RNA secondary structure. The approach was tested in cell culture separately on two different structures determined by **WALTER MOSS (PH.D. '11), SAL PRIORE (PH.D. '13, M.D. '15**), and Tian. In each case, the pair of designed mutations affected RNA splicing and reduced viral propagation, usually by more than 10-fold. The results have implications for improving vaccines made with live virus. Tian joined Turner group alums **Jim Hart (PH.D. '08, M.D. '10)** and **TIANBING XIA (PH.D. '99)** at Abbott Labs in Dallas. Jim and Tianbing have recently been promoted there.

There was also good news from other alums. Walter Moss and **ILYAS YILDIRIM (PHYSICS PH.D. '08)** 

Doug's 60th Birthday Celebration

started faculty positions at Iowa State and Florida Atlantic University, respectively. Ilyas' computational lab will be in a new building near The Scripps Research Institute where **MATT DISNEY (PH.D. '02)** is now a Professor of Chemistry. In 2015, Matt received an NIH Director's Pioneer Award for his studies on "Using a Disease-Affected Cell to Synthesize Its Own Drug." Only 13 Pioneer awards were given in 2015. Matt will be an excellent local source of advice for Ilyas.

In 2015, Doug enjoyed presenting the group's research in Turin at the annual meeting of the Italian Biophysics and Molecular Biology Society; at Telluride in an RNA Dynamics meeting; at Ohio State for a meeting on Geometric and Topological Modeling of Biomolecules; in Syracuse at the Upstate New York NMR Symposium; and in a UR Virology seminar. Seminars in 2016 were particularly enjoyable. One contributed to the celebration in Berkeley of his postdoctoral advisor, Nacho Tinoco. Unfortunately, Nacho passed only 8 months later. He lives on, however, in the hearts and minds of his many students and all who knew him. A fun visit was at Case Western Reserve, thanks to an invitation from **BLANTON TOLBERT (BIOPHYSICS** PH.D. '07). After the seminar, Blanton took Doug to a Cleveland Cavaliers - Brooklyn Nets basketball game. Despite growing up in Brooklyn, Doug rooted for the Cavs and was subsequently excited that they won the NBA championship. In November, Doug went to Warsaw, where he and Ryszard Kierzek received the AAAS/FNP Poland-US Science Award, which celebrates collaborations between Poland and the US in any area of science. This provided an opportunity to talk with diplomats from both countries and to have the experience of being separately interviewed by 4 reporters after the ceremony. Two days later in Poznan, Doug presented the group's current research to a purely scientific audience.

### **Daniel J. Weix**

Associate Professor of Chemistry



#### **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. Advances this year include continued development of our Pd/ Ni cross-Ullman reaction, improved conditions for the cross-coupling of vinyl halides with alkyl halides, a new hydrosilylation catalyst, "greener" cross-electrophile coupling, and the finding that N-hydroxyphthalimide esters act as alkyl-halides in cross-electrophile coupling. The latter development allows the use of alkanoic acids in place of alkyl halides, a major practical advance. We also have preliminary studies showing that a decarboyxlative oxidative addition can occur - a rare example of a 'new' oxidative addition step! Cross-electrophile coupling continues to mature and can now rightly be called a 'field.' In recognition of these achievements and the promise of the area, our NIH grant was renewed!

Daniel continues to teach the 'freshman organic chemistry' course and continues to find it wonderful due to the enthusiasm and talent of the students. While Dan brought demonstrations back into the lab last year, this year **DON BATESKY** helped wow the students with a multi-colored luminol demonstration and heat-sensitive



liquid crystals. Don and the students found that Dan is particularly cold-blooded: the liquid crystals refuse to react to his touch! In Chemistry 210, Dan has finally got all of the labs working well for everyone and looks forward to revising the lab manual this year.

The group was fortunate to be recognized with a variety of awards and honors this past year. Recent alumni RYAN RIBSON (B.S. '14) was a runner-up for the NSF Graduate Research Fellowship and graduate student ASTRID OLIVARES was chosen as an awardee! JILL **CAPUTO** was awarded a Departmental Travel Award in order to attend the 2016 Organic Reactions and Processes Gordon Research Conference where she presented her poster on a new, joint research direction for our group. Gordon Research Conferences are smaller meetings (usually less than 180 people) with the majority of attendees being Faculty or Scientists from industry, and presenters are selected from a large pool of applicants. Even more exciting, the organizers liked Jill's work so much that they asked her to give a talk at the meeting! Way to go Jill! KIERRA HUIHUI was selected as one of the 2016-2017 Elon Huntington Hooker Fellows in recognition of her outstanding research accomplishments. The fellowship is named in honor of Elon Huntington Hooker, a noted industrialist and Rochester alum who founded the Hooker Electrochemical Company. The awards are given annually to five graduate students in the chemical sciences, broadly defined. Kierra was also selected to attend the 2016 Organic Division Graduate Research Symposium at Bryn Mawr College this past vear.

This year we had a large amount of turnover, including five Ph.D. defenses in five months! **STEPHANIE C.M. DORN** (**RUGG**) defended her thesis in August 2016, and **YANG ZHAO** (**PH.D. '15**) defended his thesis at the beginning of October and is currently a postdoctoral fellow in the research group of Prof. Stephen Buchwald at the MIT. LUKIANA ANKA-LUFFORD (PH.D. '15) defended her thesis two weeks later and is currently a postdoctoral fellow with Prof. Arvin Das at Mt. Sinai Medical Center. In October 2015, LAURA K. G. ACKERMAN (PH.D. '15) defended her thesis before moving to Princeton, where she is currently a postdoctoral fellow with Prof. Abigail Doyle. Finally, ALEXANDER C. WOTAL (PH.D. '15) defended his thesis work in December and began a postdoc at the University of Minnesota with Prof. Ian Tonks. Finally, JILL CAPUTO (PH.D.'16) defended her thesis in December 2016 and has moved to NYC, where she is working for Porton USA. ZULEMA MELCHOR (M.S.'16), moved on to a job in the Pharmacy at the UR Medical Center, but not before she found a key result on the use of redox-active esters!

New additions to the group include first-year graduate students TARAH DIBENEDETTO, SEOYOUNG KIM and AMANDA SPIEWAK. Tarah obtained her Bachelor's degree from SUNY Oneonta in New York. Seoyoung, originally hailing from South Korea, was awarded her Bachelor's degree at Bard College, Annandale-On-Hudson in New York. Amanda, a native resident of Massachusetts, received two Bachelor's degrees, one in Chemistry and one in Forensic Science, at the University of New Haven in Connecticut. UR undergraduate ALEX CALLAHAN ('18) joined the group and is working with **KEYWAN A. JOHNSON** on cross-electrophile coupling chemistry. In addition to Alex, we also had two non-UR summer students. MARCO LOPEZ (CAL STATE LA, CLASS OF '19) was an NSF REU student and worked with Kierra Huihui on making and testing out some new CAAC ligands developed by the Bertrand group. JARED RODRIGUEZ was our first ACS SEED high school student and worked with Astrid Olivares on cross-electrophile cross-alkyl coupling. While only a junior in high school, Jared accomplished a lot. We look forward to hearing about his accomplishments in the future. Finally, two new postdoca have joined the group. DR. LIANGBIN HUANG (S. CHINA UNIV. OF TECHOLOGY) joined our group in April after spending a few years in Germany working with Prof. Lukas Gooßen at Technische Universität Kaiserslautern and **DR. MATTHEW J. GOLDFOGEL** joined the group in August after completing his Ph.D. with Prof. Simon Meek at UNC.

In other milestones, Astrid Olivares passed her oral exam and advanced to candidacy this year, and Keywan completed his third year talk. Amanda Spiewak was a class-leader for a group of middle school and high school students in the Horizons summer program at the University of Rochester this summer, a program started by Laura Ackerman a few years ago and the same program that Astrid Olivares worked with previously as well. Several group members participated in conferences and symposiums across the country. Besides the GRC and GRS mentioned above, Kierra Huihui and Astrid Olivares attended the ACS National Meeting in San Diego, CA in March of 2016.

The Weix-Wu family remains in a steady-state of five. Stella and Dan's children, Elliott (11), Madeleine (9), and Amalia (7), continue to grow, both in size and as human beings. One of their favorite new games when visiting their father is to make molecules with a model kit and ask two questions "can you make this" and "will it explode." Most recently, Elliott has joined scouts and has been messing around with both his mother's guitar and an electric bass. The girls have started learning to skateboard, something their father never really got the hang of.

In group alumni news, after a year as a visiting assistant professor at SUNY Oswego, STEPHANIE C. M. DORN (RUGG) (PH.D. '15) started as a tenure track assistant professor at Alfred State this past fall! In addition, DR. DANIEL EVERSON (PH.D. '13) joined the chemistry faculty at California State University, Chico as a tenuretrack assistant professor this fall. CHI CHEN (PH.D. '16- YALE U) took a job at Catalytic Innovations in June. ADAM HAAS (B.S. '15) took a job working at Fiabila USA. CHARLOTTE HUMES (B.A.'17) will be 'taking 5' to pursue her interests in French literature and plans to work in education. This was a break-out year for the class of 2013: DAVID GEORGE (B.S. **'13)** published his first paper with Prof. Pronin at UC-Irvine, JOE BUONOMO (B.S. '13) published his first paper with Prof. Aldrich at Univ. of Minnesota, and RACHEL KELEMEN (B.S. '13) published her first paper with Prof. Chatterjee at Boston College!



## **Senior Poster Session**



Class of 2016 Senior Thesis Poster Session 1st row: Christine Ziegler, Sarah Pristash. 2nd row: Sagar Patel, Ji Yoon Roh, Marisa Guerin, Amanda Carr, Garrick Centola, Rachel Kasimer. 3rd row: Fulei Peng, Gibran Mangui, Katherine Grasso, Aaron Balliet, Michael Moskowitz. 4th row: Murray Wan, Matthew Carbone, Christopher Melnychuk, Dylan Bleier, Richard Ladley











## Commencement

## **Bachelors and Masters Degrees Awarded in Chemistry**

### **2016 BACHELOR OF SCIENCE**

Aaron Balliet Matthew Carbone <sup>3†</sup> Amanda Carr<sup>1</sup> Garrick Centola<sup>2</sup> Katherine Grasso Marisa Guerin Rachel Kasimer<sup>1</sup> Richard Porter Ladley <sup>3</sup> Gibran Mangui Michael Moskowitz Sagar Patel Fulei Peng <sup>3\*</sup> Sarah Pristash <sup>3</sup> Ji Yoon Roh Murray Wan Christine Ziegler <sup>3†</sup>

### **2016 BACHELOR OF ARTS**

Dylan Bleier <sup>3</sup> Hai Cao Dylan Gaeta <sup>3</sup> Ping He <sup>1\*</sup> Charlotte Humes <sup>1†\*</sup> Chee Yung Kong <sup>\*\*</sup> Victoria Pu-Liang Luan <sup>1</sup> Christopher Melnychuk <sup>2</sup> Maria Mo <sup>1</sup> Katherine Neimeyer<sup>1</sup> Shane O'Neil<sup>2\*\*</sup> Anna Parker<sup>2</sup> Stephanie Salazar Hannah Slavin Kelsey Tuttle Angelo Verderame Qiuhui Wang

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



Class of 2016 Bachelor's Degree Recipients

### **2016 MASTER OF SCIENCE**

Daniel Austin Shaun Ben-Ari Rebeckah Burke Stephanie Carpenter Theresa Iannuzzi Analuz Mark Zulema Melchor Astrid Olivares Dylan Parsons

Zachary Piontkowski Paul Rubeo

# **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.

**2015:** Dylan Abrams **2016:** Matthew Carbone

### 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.

**2015:** Nicholas Hill **2016:** Rachel Kasimer

### **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.

**2015:** Kevin McClelland **2016:** Sarah Pristash

### **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.

**2015:** Lauren Weber **2016:** Fulei Peng

### **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.

**2015:** Zhijie Wu **2016:** Christine Ziegler

### **ACS Analytical Chemistry Award**

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

2015: Chitavi Maulloo

### **Chemistry Department Award**

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

### 2015

Danielle Barnett Qi Ying Li Zi Rou Liew Clayton Stumpf Nan Yang

### 2016

Dylan Gaeta Richard Porter Ladley Christopher Melnychuk

### **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.

**2015:** Chitavi Maulloo **2016:** Rachel Kasimer



### 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

Catherine Block awardee: Lauren Bolz

recommendations by the respective departments, which are evaluated by a committee appointed by the Dean of the College.

**2015:** Rachel Kasimer, Christine Ziegler **2016:** Lauren Bolz

### Ayman Amin-Salem Memorial Prize

Awarded to the member of the senior class who best displays the qualities of good character and good citizenship, such as decency, reliability, responsibility and congeniality.

### 2016: Christine Ziegler



Junior Scholar awardees: Lauren Bolz, Yifei Liang, Paul Wrona, Gavin Piester, Norman Zhao.

### **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.

### 2015

Dylan Abrams Danielle Barnett Matthew Carbone Leti Nunez

### 2016

Matthew Carbone Dylan Gaeta Richard Porter Ladley Sarah Pristash

### 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.

### 2015

Matt Carbone Dylan Gaeta Rachel Kasimer Richard Porter Ladley Fulei Peng Sarah Pristash Christine Ziegler

### 2016

Lauren Bolz Yifei Liang Gavin Piester Paul Wrona Norman Zhao

### PHI BETA KAPPA

### 2015

Dylan Abrams Danielle Barnett Nicholas Hill Qi Ying Li Chitavi Maulloo Kevin McClelland Leti Nunez Lauren Weber Zhijie Wu

### 2016

Matthew Carbone Charlotte Humes Rachel Kasimer Christine Ziegler



### 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.

### 2015

Malik Al-Afyouni Andrew Kauffmann

### 2016

Leah Frenette Miles Marnell Danielle Raymond Jennifer Urban

### **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.

**2015:** Kyle Biegasiewicz, Douglas Tusch **2016:** Kyle Rugg

### **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.

### 2015

Laura Ackerman Stephanie Daifuku Banu Kandemir Joshua Kolev Yang Zhao

### 2016

Amanda Amori Adam Feinberg Andrew Kauffmann

### **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.

### 2015

Lukiana Anka-Lufford Stephanie Dorn Adam Feinberg Jared Kneebone Gregory Pilgrim

#### 2016

Jill Caputo Banu Kandemir Jared Kneebone Lloyd Munjanja Yang Zhao

### 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.

### 2015

Rachel Carey Valerie Fleischauer Abigail Freyer Tessa Woodruff Jing Yuwen

#### 2016

Rebeckah Burke Rachel Carey Stephanie Carpenter Valerie Fleischauer Abigail Freyer Theresa Ianuzzi

### **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.

**2013-2016**: Jennifer Urban **2016-2019**: Jesse Stroka

### Agnes M. and George Messersmith Fellowship

The Agnes M. and George Messersmith Fellowship was established in 1965 and supports scholarships for graduate students in physics, chemistry, biology, and preclinical departments of the School of Medicine and Dentistry.

### 2016: Stephanie Daifuku

### **Sherman-Clarke Fellowship**

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

George Alachouzos Ningyu Liu Rachel Meyer Eric Moore Andrew Owens Dylan Parsons Jeffrey Sears Amanda Spiewak Viktoria Steck Lauren VanGelder Jade Welch

### **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.

### 2015

Rebeckah Johnson Burke Rachel Carey Abigail Freyer Analuz Mark Kyle Rugg

### 2016

Amanda Spiewak Lauren VanGelder Justin Niziol



W.D. Walters Teaching Award recipients: Amanda Spiewak, Lauren VanGelder

### **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.

### 2016: Valerie Fleischauer



Outstanding Graduate Student Award: Valerie Fleischauer
# **Student News**



Austin Bailey standing by the nanotube photonics

Congratulations to AUSTIN BAILEY, who won First Prize in the 2016 competition for the Research Initiative Award, organized by the Friends of the UR Library. This annual award recognizes excellence in undergraduate research leading towards a senior thesis, capstone project, or Physical Chemistry Institute in an independent research Heidelberg, Germany, where he project. Applicants must conducted research on carbon be full-time undergraduate students enrolled at the

University of Rochester and be interested in working towards a senior thesis, capstone project, or an independent research project. Austin will give a short presentation on his project and receive his award from the "Friends of the UR Library" in January 201 Austin was selected as a winner in the Natural & Applied Sciences section of the undergraduate writing colloquium in April 2016 for his Triplet Lifetime lab report he wrote in CHM 231. He received a cash prize and attended an awards ceremony dinner.

Austin was also chosen for an international fellowship called DAAD RISE (Research Internships in Science & Engineering) that paid his expenses to pursue a research project in carbon nanotube photonics for fourteen weeks at the Ruprecht-Karls-Universität in Heidelberg, Germany this past summer. His project focused on trying to observe strong coupling in optical microcavities fabricated with various chiralities of singlewalled carbon nanotubes. During the semester, Austin works with Dr. Todd Krauss on modifying polyfluorene derivatives for selective nanotube solubilization.



LAURA Congratulations to ACKERMAN from the Weix group! She was chosen as a finalist of the 2016 Reaxys Ph.D. Prize. Since its launch in 2010, the Reaxys PhD Prize has aimed to recognize chemistry Ph.D. students and recent graduates, fostering creativity in groundbreaking chemistry by identifying tomorrow's chemistry leaders and

empowering them to magnify the impact of their work.

Among nearly 450 applicants from around the globe, Laura was selected thanks to the remarkable originality, innovation, relevance and methodological rigor of her paper "Multimetallic Catalysed Cross-Coupling of Aryl Bromides with Aryl Triflates". She was invited to present her work at the Reaxys Prize Symposium on September 22-23 in London.

Laura was born in Honolulu, Hawaii, and grew up both in Berkeley, California and the island of Oahu. She received her BA from Claremont McKenna College in 2009, dual majoring in chemistry and religious studies, and studying abroad in Tokyo, Japan and Brighton, England. At Claremont she conducted research under the guidance of Professor Andrew W. Zanella and Professor Anna G. Wenzel, and later worked at the University of Hawaii at Manoa, learning from Professor David A. Vicic. In 2015 Laura obtained her Ph.D. from the University of Rochester, studying multimetallic catalyzed cross coupling reactions with Professor Daniel J. Weix. She is currently a Postdoctoral Fellow at Princeton University in the Doyle Research Group.



ASTRID **OLIVARES**, а second-year graduate student working in Prof. Dan Weix's lab, was selected as a 2016-2019 NSF Graduate Research Fellow. Two of our Alumni, LOUIS PAPA (now at MIT), and

KEVIN MCCLELLAND (now at Northwestern), also were selected to receive this prestigious award.

"The Graduate Research Fellowship Program is a vital part of our efforts to foster and promote excellence in U.S. science, technology, engineering and mathematics by recognizing talent broadly from across the nation," said Joan Ferrini-Mundy, NSF assistant director for Education and Human Resources. 'These awards are provided to individuals who have demonstrated their potential for significant research achievements, and they are investments that will help propel this country's future innovations and economic growth."

MATTHEW CARBONE (B.S. '16) (now at Columbia), BRITTNEY PETEL (Matson Group, UR), RYAN RIBSON (B.S. '14) (now at Caltech), JAMES SHANAHAN (B.S.'14) (now at Michigan), and LAUREN VANGELDER (Matson Group, UR) also received Honorable Mentions. Congratulations to all the awardees!

The Chemistry Department is proud to announce the completion of its fourth year participating in the **HORIZONS PROGRAM** at U of R!

The Horizons program is a six-week, full-day summer enrichment program on the University of Rochester Campus. The primary focus is to engage K-8 Rochester City School District students in meaningful and authentic learning experiences in a non-traditional school setting. The program allows students in grades K-8 to experience a summer of academic enrichment in all areas of study.

In the Chemistry Department, graduate student volunteers led by Paul Rubeo designed a series of fun

chemistry experiments to get the students excited about science. With nine chemistry themed days ranging from "Polymers" and "Colors", to "CSI-Chemistry", the students had a blast learning chemistry. It was another fun and successful summer!

Thank you to the graduate student volunteers **PAUL RUBEO** (Nilsson Group), **BRITTNEY PETEL** (Matson Group), **ANTONIO TINOCO** (Fasan Group), **AMANDA SPIEWAK** (Weix Group), and **LAUREN VANGELDER** (Matson Group).

Special thanks to Ken Simolo for providing lab coats and goggles to the students!







# Doctoral Degrees Awarded in Chemistry

#### Ph.D. Degrees Conferred on May 14, 2016

### Laura Ackerman

*Transition Metal Synergy in the Selective Formation of Carbon-Carbon Bonds* Advisor: Daniel J. Weix

# Felipe Angel

Novel Approaches to increase the Performance of Organic Photovoltaic Devices Advisor: Ching Tang

# Lukiana Anka-Lufford

Nickel-Catalyzed Reductive Coupling of Aryl Halides with Alkyl Eectrophiles Advisor: Daniel J. Weix

# Matthew Betush

Development of a recyclable chromium(II) pre-catalyst for chromium organometallic transformations Advisor: Robert K. Boeckman, Jr.

## Jonathan Chen

Two-and three-dimensional modeling of RNA structure with NMR and thermodynamics methods Advisor: Douglas H. Turner

## John Dimaio

*Functional Materials composed of Supramolecular Fibrils* Advisor: Bradley L. Nilsson

# **Christopher Favaro**

Silver Nanoparticle Films as a Light Scattering Medium for Optical Extraction Enhancement in Organic Light-emitting Diodes Advisor: Lewis Rothberg

# **Eric Henry**

A Study of Primary Collison Dynamics in Inverse-Kinematics Reaction of 78Kr on 40Ca at a Bombarding Energy of 10 MeV per Nucleon Advisor:Wolf-Udo Schröder

# Yu-Wen Huang

Studies toward the 1,6-Conjugate Addition-Initiated Nazarov Reaction Advisor: Alison J. Frontier

# **Tian Jiang**

*RNA Structure and Function of Influenza Virus* Advisor: Douglas H. Turner

# Joshua Kolev

Engineered Cytochromes P450 for the Late-stage Functionalization of Natural Products Advisor: Rudi Fasan

## Wathsala G.H.M. Liyanage

Amyloid-inspired amino acid based functional hydrogel materials: structural insights Advisor: Bradley L. Nilsson

# **Benjamin Martin**

*Conjugated Polymer Studies: Still Some Surprises Left* Advisor: Lewis Rothberg

## Sarah Paulson

Studies of the Catalytic Mukaiyama Aldol Reaction Utilizing Chiral Oxazaborolidines: Application to the Synthesis of Substituted Butenolides Advisor: Robert K. Boeckman, Jr.

## **Gregory A. Pilgrim**

*Electrons, Protons, and Solvents in Carbon Nanotubes* Advisor: Todd D. Krauss

## Stefanie Rugg (Dorn)

Nickel-Catalyzed Reductive Coupling with Michael Acceptors Advisor: Daniel J. Weix

## **Randy Sabatini**

Excited State Dynamics, Molecular Interactions, and Electron Transfer in Systems for the Photochemical Production of Hydrogen Advisor: Richard Eisenberg, David McCamant

# Terrell Samoriski

The Design, Implementation and Evaluation of Peer-Led Team Learning (PLTL) in a Second Semester Organic Laboratory Course Advisor: Joseph P. Dinnocenzo

## **Aaron Walsh**

*Transition Metal-Mediated Carbon-Heteroatom Bond Activation* Advisor: William D. Jones

# Hsiu-Ying (Helen) Wei

Colloidal Semiconductor Quantum Dots with Tunable Surface Composition Advisor: Todd D. Krauss

### **Millard Wyman**

Kinetics of Charge Recombination in a Ladder Phenylene Polymer Advisor: Lewis Rothberg

# Xiaoju Zhang

Computational Studies of Yeast Protein Translational Components Advisor: David Matthews

## Yang Zhao

Nickel-Catalyzed Reductive Coupling of Epoxides and Aziridines Advisor: Daniel J. Weix

#### Ph.D. Degrees Conferred on August 31, 2016

## Malik Al-Afyouni

The Coordination Chemistry and Reactivity of Organometallic Cobalt, Iron, and Manganese Complexes Advisor: Michael L. Neidig

## Kathlyn Fillman

Theoretical and Spectroscopic Studies of Mid-First Row Transition Metal Complexes Advisor: Michael L. Neidig

# Lloyd Munjanja

Transition Metal Hydrides (M-H) Facilitating Carbon - Sulfur, Carbon - Carbon Bonds Activation and Alkene Isomerization Advisor: William D. Jones

## Amanda Preske

Programmed Synthesis of Metal Chalcogenide Semiconductor Nanocrystals Using Secondary Phosphines Advisor: Todd D. Krauss

## Matthew Sharpe

On the interaction of tritium with the surfaces of aluminum, copper, stainless steel (type 316), and gold Advisor: Wolf-Udo Schröder

## **Alexander Wotal**

Nickel-Catalyzed Ketone Formation and Stoichiometric Reactivity of Nickel(II) Acyl Halide Species with Organic Halides Advisor: Daniel J. Weix

#### Ph.D. Degrees Conferred on October 7, 2016

## Annada Rajbhandary

Investigating the Relationship Between Structure and Self-Assembling Behavior of Fmoc-Protected Phenylalanine Derivatives Advisor: Bradley L. Nilsson

#### **Kelly Sowers**

Synthesis, Photophysics, and Applications of Colloidal Semiconductor Quantum Dots Advisor: Todd D. Krauss

#### Ph.D. Degrees Conferred on December 31, 2016

#### **Kyle Biegasiewicz**

I. Mechanistic Studies, Optimization, and Further Applications of the Organocatalytic Alpha -Hydroxymethylation of Aldehydes II. Studies Toward the Total Synthesis of FK-506 Advisor: Robert K. Boeckman, Jr.

#### Banu Kandemir

*Electrocatalytic Proton Reduction from Water by Biomolecular Cobalt Catalysts* Advisor: Kara Bren

# **Postdoctoral Fellows**

Farnaz Alipour Shakib Prof. Huo **(2016)** University of Alberta, Edmonton, Canada

Ivan de Paola Prof. Fasan **(2015)** IBB-CNR, Napoli, Italy

Matthew Goldfogel Prof. Weix (2016) University of North Carolina, Chapel Hill, NC

**Bing Gu** Profs. Fasan & Franco **(2016)** University of South Carolina

**Cassandra Hayes** Prof. Jones **(2013)** Simon Fraser University, Burnaby, BC

Liangbin Huang Prof. Weix (2016) South China University of Technology, Guang Zhou, China

Feng Li Prof. Matson **(2015)** University of Notre Dame Guocan Li Prof. Eisenberg (2016) Florida State University

Hongjin Lv Prof. Eisenberg (2015) Emory University

Salvadore Munoz Prof. Neidig (2015) University of Indiana, Bloomington, IN

Phuong Quoc Thuc Nguyen Prof. Fasan (2013) Nanyang Technological University, Singapore

**Gopeekrishnan Sreenilayam** Prof. Fasan **(2011)** University of Iowa, Iowa City, IA

Venkat Srinivasan Prof. Boeckman (2016) University of Rochester, Rochester, NY

Sharma SRK Chaitanya Yamijala Prof. Huo (2016) JNCASR, Bangalore, India



# Faculty Publications July 2015 - December 2016

## **ROBERT K. BOECKMAN, JR.**

Organocatalytic Enantioselective α-Hydroxymethylation of Aldehydes: Mechanistic Aspects and Optimization. R.K. Boeckman, Jr., K.F. Biegasiewicz, D.J. Tusch, J.R. Miller, *J Org Chem*, **2015**, *80*, 4030.

(S)-1,1-Diphenylprolinol Trimethylsilyl Ether. R.K. Boeckman Jr., D.J. Tusch, and K.F. Biegasiewicz, *Org Synth*, **2015**, *92*, 309-319.

Organocatalyzed Direct Asymmetric α-Hydroxymethylation of Aldehydes. R.K. Boeckman Jr., D.J. Tusch, K.F. Biegasiewicz, *Org Synth*, **2015**, *92*, 320.

A Scalable Total Synthesis of (-)- Nakadomarin A. R.K. Boeckman, Jr., H. Wang, K.W. Rugg, N.E. Genung, K. Chen, T.R. Ryder, *Organic Letters*, **2016**, *18*, 6136.

# **KARA L. BREN**

Discovery of the magnetic behavior of hemoglobin: A beginning of bioinorganic chemistry. K.L. Bren, R. Eisenberg, H.B. Gray, *Proc Natl Acad Sci USA*, **2015**, *112*, 13123.

Going with the Electron Flow: Heme Electronic Structure and Electron Transfer in Cytochrome c. K.L. Bren, *Isr J Chem*, **2016**, *56*, 693. (Special issue in celebration of Harry Gray's 80<sup>th</sup> birthday)

Semisynthetic and Biomolecular Hydrogen Evolution Catalysts.B. Kandemir, S. Chakraborty, Y. Guo, K.L. Bren, *Inorg Chem*,2016, 55, 467. (Article in Forum on Small Molecule Activation: From Biological Principles to Energy Applications)

Hydrogen Evolution from Water under Aerobic Conditions Catalyzed by a Cobalt ATCUN Metallopeptide. B. Kandemir, L. Kubie, Y. Guo, B. Sheldon, K.L. Bren, *Inorg Chem*, **2016**, *55*, 1355. (Featured on journal cover and selected as ACS Editor's Choice.)

NMR Analysis of Spin States and Spin Densities, in *Spin States in Biochemistry and Inorganic Chemistry: Influence on Structure and Reactivity.* K.L. Bren; Edited by M. Swart and M. Costas, John Wiley & Sons, Ltd, Chichester, United Kingdom (2016).

Extracellular Electron Transfer on Sticky Paper Electrodes: Carbon Paste Paper Anode for Microbial Fuel Cells. P. Lamberg, K.L. Bren, *ACS Energy Letters*, **2016**, 1(5), 895.

# **RICHARD EISENBERG**

Light-driven generation of hydrogen: New chromophore dyads for increased activity based on Bodipy dye and Pt(diimine) (dithiolate) complexes. B. Zheng, R.P. Sabatini, W.-F. Fu, M.-S. Eum, W.W. Brennessel, L. Wang, D.W. McCamant, R. Eisenberg, *Proc Natl Acad Sci USA*, **2015**, *112*, E3987.

Discovery of the magnetic behavior of hemoglobin: A beginning of bioinorganic chemistry. K.L. Bren, R. Eisenberg, H.B. Gray, *Proc Natl Acad Sci USA*, **2015**, *112*, 13123.

Efficient Bimolecular Mechanism of Photochemical Hydrogen Production Using Halogenated Boron-Dipyrromethene (Bodipy) Dyes and a Bis(dimethylglyoxime) Cobalt(III) Complex. R.P. Sabatini, B. Lindley, T.M. McCormick, T. Lazarides, W.W. Brennessel, D.W. McCamant, R. Eisenberg, *J Phys Chem B*, **2016**, *120*, 527.

Catalytic Light-Driven Generation of Hydrogen from Water by Iron Dithiolene Complexes. H. Lv, T. P. Ruberu, V. E. Fleischauer, W. W. Brennessel, M. L. Neidig, R. Eisenberg, J Am Chem Soc, 2016, 138, 11654.

A Comparative Study of the Photophysics of Phenyl, Thienyl, and Chalcogen Substituted Rhodamine Dyes. R.P. Sabatini, M.F. Mark, D.J. Mark, M.W. Kryman, J.E. Hill, W.W. Brennessel, M.R. Detty, R. Eisenberg, D.W. McCamant, *Photochem & Photobiol Sci*, **2016**, *15*, 1417.

Chromophoric Dyads for the Light-Driven Generation of Hydrogen: Investigation of Factors in the Design of Multicomponent Photosensitizers for Proton Reduction. P.-Y. Ho, B. Zheng, D. Mark, W.-Y. Wong, D.W. McCamant, R. Eisenberg, *Inorg Chem*, **2016**, *55*, 8348.

# **SAMIR FARID**

Spontaneous polarization induced electric field in zinc oxide nanowires and nanostars. S. Farid, M. Choi, D. Datta, M.A. Stroscio, M. Dutta, *J Appl Phys*, **2016**, *119*, 16.

Enhanced optical properties due to indium incorporation in zinc oxide nanowires. S. Farid, S. Mukherjee, K. Sarkar, M. Mazouchi, M.A. Stroscio, M. Dutta, *Appl Phys Lett*, **2016**, *108*, 2.

# **JAMES M. FARRAR**

Ion-Molecule Reaction Dynamics: Velocity Map Imaging Studies of N+ and O+ with  $CD_3OD$ . L. Pei, J.M. Farrar, *J Chem Phys*, **2015**, *143*, 084304.

Velocity Map Imaging Study of Ion-Radical Chemistry: Charge Transfer and Carbon-Carbon Bond Formation in the Reactions of Allyl Radicals with C+. L. Pei, J.M. Farrar, *J Phys Chem A*, **2016**, *120*, 6122.

Angular and Energy Distribution of Fragment Ions in Dissociative Double Photoionization of Acetylene and the 31.9 – 50.0 eV Photon Energy Range. S. Falcinelli, M. Alagia, J.M. Farrar, K.S. Kalogerakis, F. Pirani, R. Richter, L. Schio, S. Stranges, M. Rosi, and F. Vecchiocattivi, *J Chem Phys*, **2016**, *145*, 114308.

#### **RUDI FASAN**

Synthesis of Macrocyclic Organo–peptide Hybrids from Ribosomal Polypeptide Precursors via CuAAC-Hydrazide-Mediated Cyclization. J.M. Smith, R. Fasan, *Meth Mol Biol*, **2015**, *1248*, 23.

Side-chain-to-tail cyclization of ribosomally derived peptides promoted by aryl and alkyl amino-functionalized unnatural amino acids. J.R. Frost, Z. Wu, Y.C. Lam, A.E. Owens, R. Fasan, *Org Biomol Chem*, **2016**, *14*, 5803.

Aldehyde and Ketone Synthesis by P450-Catalyzed Oxidative Deamination of Alkyl Azides. S. Giovani, H. Alwaseem, R. Fasan, *ChemCatChem*, **2016**; 8, 2609.

Efficient conversion of primary azides to aldehydes catalyzed by active site variants of myoglobin. S. Giovani, R. Singh, R. Fasan, *Chem Sci*, **2016**, *7*, 234.

Chemoenzymatic synthesis and antileukemic activity of novel C9- and C14-functionalized parthenolide analogs. V. Tyagi, H. Alwaseem, Q.Y. Li, K.M. O'Dwyer, J. Ponder, C.T. Jordan, R. Fasan, *Bioorg Med Chem*, **2016**, *24*, 3876.

Myoglobin-Catalyzed Olefination of Aldehydes. V. Tyagi, R. Fasan, *Angew Chem Int Ed*, **2016**, *55*, 2512.

Biocatalytic synthesis of allylic and allenyl sulfides through a myoglobin-catalyzed Doyle-Kirmse reaction. V. Tyagi, G. Sreenilayam, P. Bajaj, A. Tinoco, R. Fasan, *Angew Chem Int Ed*, **2016**, *55(43)*, 13562.

Gram-scale synthesis of chiral cyclopropane-containing drugs and drug precursors using engineered myoglobin catalysts with complementary stereoselectivity. P. Bajaj, G. Sreenilayam, V. Tyagi, R. Fasan, *Angew Chem Int Ed*, **2016**, 55(52): 16110.

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

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#### **IGNACIO FRANCO**

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## **TODD D. KRAUSS**

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#### **DAVID W. MCCAMANT**

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## **BRADLEY L. NILSSON**

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#### W. UDO SCHRÖDER

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#### **DOUGLAS H. TURNER**

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### **DANIEL J. WEIX**

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# Seminars & Colloquia

# **AUGUST 2015**

Stephanie Rugg (Dorn) (University of Rochester, Department of Chemistry) "Nickel-Catalyzed Reductive Coupling with Michael Acceptors" August 4, 2015 (Ph.D. Defense)

Aaron Walsh (University of Rochester, Department of Chemistry) "Transition Metal-Mediated Carbon-Heteroatom Bond Activation" August 14, 2015 (Ph.D. Defense)

Matthew Betush (University of Rochester, Department of Chemistry) "Development of a recyclable chromium(II) pre-catalyst for chromium organometallic transformations" August 19, 2015 (Ph.D. Defense)

Joshua Kolev (University of Rochester, Department of Chemistry) "Engineered Cytochromes P450 for the Late-stage Functionalization of Natural Products" August 21, 2015 (Ph.D. Defense)

# **SEPTEMBER 2015**

Professor Vasilii Petrenko (University of Rochester, Earth and Environmental Sciences) "Using carbon-14 to investigate the response of natural methane emissions to global warming" September 9, 2015

Dr. Gary Dombrowski (The Dow Chemical Company, Dow Advanced Materials) "Theoretical and Practical Elements of Emulsion Polymerization" September 11, 2015

Christopher Favaro (University of Rochester, Department of Chemistry) "Silver Nanoparticle Films as a Light Scattering Medium for Optical Extraction Enhancement in Organic Light-Emitting Diodes" September 11, 2015 (Ph.D. Defense)

Professor Suzanne Blum (University of California - Irvine, Department of Chemistry) "Aminoboration and Oxyboration Reactions" September 18, 2015

# Victor J. Chambers Memorial Lecture



Professor Andrei K. Yudin (University of Toronto, Department of Chemistry)

"In search of biologically active compounds using the tools of chemical synthesis" September 21, 2015

"Amphoteric aziridine aldehydes" September 22, 2015

"New directions in organoboron chemistry" September 23, 2015

Tian Jiang (University of Rochester, Department of Chemistry) "RNA Structure and Function of Influenza Virus" September 23, 2015 (Ph.D. Defense)

Professor Randall Goldsmith (University of Wisconsin - Madison, Department of Chemistry) "Adventures in Single-Molecule Spectroscopy: Optical Microresonators and Mechanistic Organometallic Chemistry" September 28, 2015

# **OCTOBER 2015**

Yang Zhao (University of Rochester, Department of Chemistry) "Nickel-Catalyzed Reductive Coupling of Epoxides and Aziridines" October 2, 2015 (Ph.D. Defense)

**Professor Haitao Liu (University of Pittsburgh, Department of Chemistry)** "On the Intrinsic Wettability of Graphene and Graphite" October 5, 2015

Professor John P. Richard (University at Buffalo, Department of Chemistry) "The Architecture of Enzyme Dianion Activation Sites" October 9, 2015

Professor Hao Xu (Georgia State University, Department of Chemistry) "Searching for New Reactivity: Iron-Catalyzed Stereoselective Olefin Aminohydroxylation and Aminofluorination Reactions" October 16, 2015 Lukiana Anka-Lufford (University of Rochester, Department of Chemistry) "Nickel-Catalyzed Reductive Coupling of Aryl Halides with Alkyl Electrophiles" October 19, 2015 (Ph.D. Defense)

Professor R.J.M. Klein Gebbink (Utrecht University - The Netherlands, Department of Chemistry) "Playing around with oxygen: homogeneous catalysts for the incorporation and removal of oxygen functionalities from biomass" October 21, 2015

Laura Ackerman (University of Rochester, Department of Chemistry) "Transition Metal Synergy in the Selective Formation of Carbon-Carbon Bonds" October 26, 2015 (Ph.D. Defense)

Professor David Vicic (LeHigh University, Department of Chemistry) "Organometallic Aspects of Alkyl and Fluoroalkyl Cross-Coupling Reactions" October 27, 2015

# Joint Optics, Chemistry, and Materials Science Colloquium



Professor Harry A. Atwater (California Institute of Technology, Applied Physics and Materials Science) "Electronically Tunable Metamaterials and Metasurfaces" October 28,

John DiMaio (University of Rochester, Department of Chemistry) "Functional Materials Composed of Supramolecular Fibrils" October 30, 2015 (Ph.D. Defense)

2015

# **NOVEMBER 2015**

Professor Lai-Sheng Wang (Brown University, Department of Chemistry) "Photoelectron Spectroscopy of Size-Selected Boron Clusters: From Planar Structures to Borophenes and Borospherenes" November 2, 2015 Professor Richard E. Partch (Clarkson University, Department of Chemistry) "Colloids for Medical Therapy : Chemical Overdose Application" November 6, 2015

Professor Marion Emmert (Worcester Polytechnic Institute, Departments of Chemistry & Biochemistry, Chemical & Mechanical Engineering) "Breaking Strong Bonds and Recovering Rare Earths: Adventures in Sustainable Chemistry" November 9, 2015

Professor Jennifer Prescher (University of California - Irvine, Department of Chemistry) "Expanding the imaging toolbox" November 13, 2015

Xiaoju Zhang (University of Rochester, Department of Chemistry) "Computational Studies of Yeast Protein Translational Components" November 13, 2015 (Ph.D. Defense)

Professor Andrew Greytak (University of South Carolina, Department of Chemistry and Biochemistry) "Quantum Dot Purification and Metrics for Rational Control of Shell Growth, Ligand Exchange, and Quantum Yield" November 16, 2015

Professor Poul Petersen (Cornell University, Department of Chemistry and Chemical Biology) "Structure and ultrafast vibrational dynamics of strongly hydrogen-bonded complexes" November 23, 2015

Professor David Blank (University of Minnesota, Department of Chemistry) "Exciton Dynamics in Organic Solar Cells" November 30, 2015

# **DECEMBER 2015**

Alexander Wotal (University of Rochester, Department of Chemistry) "Nickel-Catalyzed Ketone Formation and Stoichiometric Reactivity of Nickel(II) Acyl Halide Species with Organic Halides" December 3, 2015 (Ph.D. Defense)

Millard Wyman (University of Rochester, Department of Chemistry) "Kinetics of Charge Recombination in a Ladder Phenylene Polymer" December 7, 2015 (Ph.D. Defense)

Professor Ruth Webster (University of Bath UK, Department of Chemistry) "Exploring iron catalysed phosphine synthesis: from hydrophosphination to dehydrocoupling" December 7, 2015 Professor Ratmir Derda (University of Alberta, Canada, Department of Chemistry and Alberta Glycomics Centre) "Discovery of Functional Ligands from Genetically-Encoded Libraries of Peptide Derivatives" December 11, 2015

# **JANUARY 2016**

Joseph Barendt, Ph.D. (Chiral Technologies, Inc.) "The Quest for Single Enantiomer Pharmaceuticals" January 15, 2016

Jerzy Klosin, Ph.D. (Dow Chemical Company) "Development of Molecular Catalysts for the Production of Ethylene-Based Copolymers" January 18, 2016

Kyle Rugg (University of Rochester, Department of Chemistry) "Mechanistic and Synthetic Studies of the Himbert Intramolecular Arene/Allene Diels-Alder Cycloaddition" January 22, 2016

Jennifer Urban (University of Rochester, Department of Chemistry) "Super-Resolution Biological Imaging Using Quantum Dots" January 25, 2016

Professor Emily Weiss (Northwestern University, Department of Chemistry) "Energy Transfer in Solution-Phase Quantum Dot-Molecule and Quantum Dot-Quantum Dot Assemblies" January 27, 2016

Tamas Benkovics, Ph.D. (Bristol-Myers Squibb Process Chemistry, New York, New York) "Stereoselective Synthesis of Nucleoside Reverse Transcriptase Inhibitor (NRTI) BMS-986001" January 29, 2016

# **FEBRUARY 2015**

Professor Jason Benedict (State University of New York at Buffalo, Department of Chemistry) "Watching crystals work: Structural dynamics of metalorganic frameworks" February 1, 2016

Miao-Ping Chien, Ph.D. (Harvard University, Department of Chemistry and Chemical Biology) "Responsive Molecules for Biology" February 8, 2016

Professor Christopher M. Yakacki (University of Colorado Denver, Department of Mechanical

**Engineering)** "Main-Chain Liquid-Crystalline Elastomers Using a Two-Stage Thiol-Acrylate Reaction" February 10, 2016 Eric Stoutenburg (University of Rochester, Department of Chemistry) "Development and Mechanistic Studies of Rhodium Catalyzed Alkene Hydroacylation" February 19, 2016

# Dr. Ralph Ernstorfer (Fritz-Haber Institute of the Max Planck Society, Department of Physical

**Chemistry)** "Electronic and Structural Dynamics in Solids: from electron-phonon coupling to spin- and pseudospinpolarized excited states" February 22, 2016

Professor Andy Borovik (University of California, Irvine, Department of Chemistry) "Synthetic Chemistry as a Window into Biology: Architectural Complexity at the Molecular Level" Februrary 24, 2016

Pat Harrington (University of Rochester, Department of Chemistry) "Development of a Gold Multifaceted Catalysis Approach to the Synthesis of Highly Substituted Pyrroles" February 26, 2016

Professor Dustin Froula (University of Rochester, Laboratory for Laser Energetics) "Raman Amplification of High Power Laser Pulses" Februrary 29, 2016

# **MARCH 2015**

Amanda Amori (University of Rochester, Department of Chemistry) "Photophysical Studies of Polymer Enriched Single-Walled Carbon Nanotubes" March 7, 2016

Matthew Goldfogel (University of North Carolina, Chapel Hill, Department of Chemistry) "Hydrofunctionalization via Electrophilic Alkene Activation: Introducing Carbodicarbenes as Catalytically Active Ligands" March 9, 2016

Yu-Wen Huang (University of Rochester, Department of Chemistry) "Studies toward the 1,6-Conjugate Addition-Initiated Nazarov Reaction" March 17, 2016(Ph.D. Defense)

Professor Andrew White (University of Rochester, Department of Chemical Engineering) "Teaching Numerical Methods and Statistics with Web-based Interactive Computing" March 21, 2016

Professor Matthew Bogyo (Stanford University School of Medicine, Department of Pathology) "New chemical probe technologies: applications to cancer imaging and drug discovery" March 23, 2016 Keywan Johnson (University of Rochester, Department of Chemistry) "Mechanism of the Platinum(II)-Catalyzed Hydroamination of 4-Pentenylamines" March 25, 2016

Amanda Preske (University of Rochester, Department of Chemistry) "Programmed Synthesis of Metal Chalcogenide Semiconductor Nanocrystals Using Secondary Phosphines" March 25, 2016(Ph.D. Defense)

Professor Gordana Dukovic (University of Colorado, Boulder, Department of Chemistry and Biochemistry) "Photophysics and photochemistry of nanoscale semiconductors and implications for solar fuel generation" March 28, 2016

Professor John Slattery (University of York-UK, Department of Chemistry) "C-F bond formation in organometallic complexes via outer-sphere electrophilic fluorination" March 30, 2016

Benjamin Martin (University of Rochester, Department of Chemistry) "Conjugated Polymer Studies: Still Some Surprises Left" March 30, 2016(Ph.D. Defense)

# **APRIL 2015**

**Professor Dean Tantillo (University of California, Davis, Department of Chemistry)** "Walking in the Woods with Quantum Chemistry - The Importance of Inherent Carbocation Reactivity in Terpene Biosynthesis" April 1, 2016

**Tessa Baker (University of Rochester, Department of Chemistry)** "Insight into carbene containing pincers from well defined complexes to in situ reactions." April 4,2016

Professor Jeffery Byers (Boston College, Department of Chemistry) "Iron-Based Catalysts for the Diversification of a Biodegradable Polymer" April 5, 2016

Professor William Wuest (Temple University, Department of Chemistry) "Draining the Moat: A Natural Product-Inspired Approach to Combat Bacterial Biofilms" April 8, 2016

Professor Eunsuk Kim (Brown University, Department of Chemistry) "Synthetic Modeling Chemistry of Iron-Sulfur Clusters in NO Signaling" April 11, 2016

#### Morris Bullock, Ph.D. (Pacific Northwest National

**Laboratory)** "Design of Molecular Electrocatalysts for the Production and Oxidation of Hydrogen: Shoving Protons Around With Proton Relays" April 13, 2016

**Professor Amber Krummel (Colorado State University, Department of Chemistry)** "Illuminating the Structure of Dye Molecules in the Condensed Phase with Nonlinear Optical Spectroscopy" April 18, 2016

Andrew Owens (University of Rochester, Department of Chemistry) "Chemical genetic strategies for the identification of AMP-activated protein kinase substrates." April 22, 2016

**Professor Eric Schelter (University of Pennsylvania, Department of Chemistry)** "Metals Recycling and Photoredox: New Chemistry to Improve the Sustainability of the Rare Earth Elements" April 25, 2016

# **MAY 2015**

Matthew Sharpe (University of Rochester, Department of Chemistry) "On the interaction of tritium with the surfaces of aluminum, copper, stainless steel (type 316), and gold" May 3, 2016 (Ph.D. Defense)

# **Hutchison Memorial Lecture**



Professor Guy Bertrand (University of California, San Diego, Department of Chemistry)

"From useless to useful stable carbenes." May 2, 2016

"CAACs as powerful tools in organic, inorganic and organometallic chemistry" May

3, 2016

"The novel generation of stable carbenes and related species." May 4, 2016

Hanan Alwaseem (University of Rochester, Department of Chemistry) "Artificial Metalloenzymes Based on Biotin-Avidin Technology" May 6, 2016

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Professor Lars Gundlach (University of Delaware, Departments of Chemistry and Bio-chemistry, Physics and Astronomy) "Ultrafast Charge Carrier Dynamics in Solar Energy Relevant Materials" May 10, 2016

Abigail Freyer (University of Rochester, Department of Chemistry) "Charge Properties of Doped Semiconductor Nanocrystals" May 11, 2016

**Oliver Swart (University of Rochester, Department of Chemistry)** "Increasing the Utility of Stapled Peptides Through Novel Linker Chemistries" May 13, 2016

Saikat Chakraborty and Jianbo Zhao (University of Rochester, Department of Chemistry) "1: Bio-molecular systems for solar hydrogen generation; 2: Approaches to Improving Prediction of RNA 3D Structures Using Molecular Dynamics" May 16, 2016

# **Biological Chemistry Cluster Retreat** Seminar

Professor Thomas Kodadek (Scripps Research Institute, Florida Campus) "Chemical tools to monitor and manipulate the proteome" May 19, 2016

Valerie Fleischauer and Sreyoshi Sur (University of Rochester, Department of Chemistry) "1: Active Species and Mechanism in Alkyl-Alkyl Cross-Coupling with Iron ; 2: Insights into the mechanism of fengycin, an antimicrobial lipopeptide" May 23, 2016

Jing Yuwen (University of Rochester, Department of Chemistry) "Homogeneous hydrogenation of carbon dioxide to methanol" May 25, 2016

John McAnany (University of Rochester, Department of Chemistry) "Amelioration of a Disease State by Small-Molecule RNA Splicing Modulators" May 27, 2016

# **JUNE 2016**

#### Jade Welch (University of Rochester, Department

of Chemistry) "Modifications of Plant Viruses for Enhanced Drug Delivery" June 10, 2016

Lloyd Munjanja (University of Rochester, Department of Chemistry) "Transition Metal Hydrides (M-H) Facilitating Carbon - Sulfur, Carbon - Carbon Bonds Activation and Alkene Isomerization" June 15, 2016(Ph.D. Defense)

Leah Frenette (University of Rochester, Department of Chemistry) "Rediscovering Active Precursors in CdSe Nanocrystal Synthesis" June 20, 2016

Kelly Sowers (University of Rochester, Department of Chemistry) "Synthesis, Photophysics, and Applications of Colloidal Semiconductor Quantum Dots" June 23, 2016(Ph.D. Defense)

Kathlyn Fillman (University of Rochester, Department of Chemistry) "Theoretical and Spectroscopic Studies of Mid-First Row Transition Metal Complexes" June 27, 2016(Ph.D. Defense)

Malik Al-Afyouni (University of Rochester, Department of Chemistry) "The Coordination Chemistry and Reactivity of Organometallic Cobalt, Iron, and Manganese Complexes" June 27, 2016(Ph.D. Defense)

# **JULY 2016**

Annada Rajbhandary (University of Rochester, Department of Chemistry) "Investigating the Relationship Between Structure and Self-Assembling Behavior of Fmoc-Protected Phenylalanine Derivatives" July 21, 2016 (Ph.D. Defense)

# **AUGUST 2016**

Professor R.Tom Baker (University of Ottawa-Canada, Department of Chemistry and Biomolecular Sciences) "Iron Casting Call: Fe Thiolate and Amido Catalysts Featuring Hemilabile SNS Ligands"

August 16, 2016

Stephanie Daifuku (University of Rochester, Department of Chemistry) "Insight into Iron C-C Cross-Coupling Catalysis through Structure, Bonding and Mechanism" August 16, 2016(Ph.D. Defense)'

# **SEPTEMBER 2016**

Professor Samir Zard (Ecole Polytechnique -France, Laboratoire de Synthèse Organique) "A Radical Solution to an Old Problem. Some New Perspectives for Organic Synthesis" September 7, 2016

Professor Igor Alabugin (Florida State University, Department of Chemistry and Biochemistry) "Choreographing cyclizations and fragmentations in radical cascades" September 9, 2016

Zhi Li and Michael Mark (University of Rochester, Department of Chemistry) "I. Towards Modeling Single Molecule Pulling Coupled to Transport, II. Ultrafast Dynamics of Chromophores having Potential use for Solar Hydrogen Production" September 12, 2016

Banu Kandemir (University of Rochester, Department of Chemistry) "Electrocatalytic Proton Reduction from Water by Biomolecular Cobalt Catalysts" September 13, 2016(Ph.D. Defense)

Professor Chris Vanderwal (University of California, Irvine, Department of Chemistry) "Analogue-Oriented Synthesis Strategies to Address Bioactive Natural Product Families" September 14, 2016

Jill Caputo (University of Rochester, Department of Chemistry) "I. Nickel-Catalyzed Additions to Imines and Aldehydes and II. Photoredox Catalysis with Quantum Dot Catalysts in Carbon-Carbon Bond Forming Reactions" September 15, 2016(Ph.D. Defense)

# Andrew S.Kende Distinguished Lecture



### Professor Colin Nuckolls (Columbia University. Department of Chemistry)

"Contorted Aromatics as Components in Electronic Materials" September 19, 2016

"Single Molecule Electronics" September 20, 2016

"Superatoms as building blocks for Materials" September 21, 2016

# Professor Matthew Liptak (University of Vermont,

**Department of Chemistry)** "Novel Functions from Dynamic Motions" September 26, 2016

Rachel Carey (University of Rochester, Department of Chemistry) "Electron Transport Through Molecules: Toward Accurate and Efficient Large Scale Simulations" September 28, 2016

# **Special Inorganic Seminar**

Professor Simon Duckett (The University of York -England, Department of Chemistry) "Parahydrogen Induced Polarization in NMR Spectroscopy and Imaging" September 29, 2016

# **Seymour Rothchild Lecture**

Professor Jacqueline K. Barton (California Institute of Technology, Division of Chemistry) "DNA Signaling" September 30, 2016

# **OCTOBER 2016**

**Professor Kyle Lancaster (Cornell University, Department of Chemistry and Chemical Biology)** "Mechanistic and Electronic Structural Insights into the Metallobiochemistry of Nitrification" October 3, 2016

Professor Abraham Nitzan (University of Pennsylvania, Department of Chemistry) "Molecular conduction and beyond" October 5, 2016

Kyle Biegasiewicz (University of Rochester, Department of Chemistry) "I. Mechanistic Studies, Optimization, and Further Applications of the Organocatalytic alpha -Hydroxymethylation of Aldehydes II. Studies Toward the Total Synthesis of FK-506" October 5, 2016(Ph.D. Defense)

**Professor Jared Lewis (University of Chicago, Searle Chemistry Laboratory)** "Engineering Proteins for Selective Catalysis" October 7, 2016

**Professor Libai Huang (Purdue University, Department of Chemistry)** "Ultrafast Nanoscopy of Energy and Charge Transport" October 10, 2016 Professor Charles Jakobsche (Clark University, Department of Chemistry and Biochemistry) "From Organic Synthesis to Chemical Biology" October 14, 2016

Professor Joshua Vura-Weis (University of Illinois at Urbana-Champaign, Department of Chemistry) "Shrinking the Synchrotron: Ultrafast Tabletop XANES of Transition Metal Complexes and Organohalide Perovskites" October 17, 2016

Professor Nancy Makri (University of Illinois at Urbana–Champaign, Department of Chemistry) "Quantum-Classical Path Integral Simulation of Condensed Phase Dynamics" October 19, 2016

**Professor Neal Mankad (University of Illinois at Chicago, Department of Chemistry)** "Catalytic Transformations That Utilize Bimetallic Cooperation" October 20, 2016

# W. Albert Noyes Jr. Memorial Lecture



Professor Richard Zare (Stanford University, Department of Chemistry) "Microdroplet Chemistry" October 25, 2016

Professor Sylviane Sabo-Etienne (French National Center for Scientific Research (CNRS), Laboratoire de Chimie de Coordination (LCC)) "Mechanistic Studies on Polyhydride-Catalyzed Transformations" October 26, 2016

# **NOVEMBER 2016**

Professor Laurel L. Schafer (University of British Columbia, Department of Chemistry) "Developing Early Transition Metal Complexes for the Catalytic Synthesis of Amine" November 2, 2016 Professor Jeff Aubé (University of North Carolina, Eshelman School of Pharmacy) "Reflections on a Decade of Library Construction" November 4, 2016

Professor Frank Spano (Temple University, Department of Chemistry) "Short and Long-range Excitonic Coupling in Molecular Aggregates: A New Paradigm for Designing Organic Electronic Materials"

November 7, 2016

Professor Thomas B. Rauchfuss (University of Illinois at Urbana-Champaign, School of Chemical Sciences) "How Hydrogen is Made Naturally" November 9, 2016

Professor Latha Venkataraman (Columbia University, Department of Applied Physics) "Physics and Chemistry of Single-Molecule Circuits" November 14, 2016

Professor Michael Neidig (University of Rochester, Department of Chemistry) "Structure, Bonding and Mechanism in Iron-Catalyzed Cross-Coupling" November 30, 2016

# **DECEMBER 2016**

# **CCHF Virtual Symposium Speakers**

Professor Donna Blackmond (Scripps Research Institute, Florida Campus) "Kinetic Studies in Support of Mechanistic Analysis in C-H Functionalization Reactions" December 13, 2016

**Professor Matthew Gaunt (University of Cambridge)** "Catalytic C-H activation of aliphatic amines" December 13, 2016

**Professor Justin Du Bois (Stanford University)** "Selective Oxidation of C-H Bonds with Hyper-Electrophiles" December 13, 2016

**Professor Paul Chirik (Princeton University)** "Cobalt-Catalyzed C(sp2)-H and C(sp3)-H Bond Functionalization" December 13, 2016

Dr. Han Xiao (Stanford University, Department of Chemistry) "Precision Glycocalyx Editing for Cancer Immunotherapy" December 15, 2016

# **Staff News**

The staff enjoyed their annual summer outing on the Colonial Belle. It was a beautiful day- no rain this time!

# ADMINISTRATIVE STAFF

**DEB CONTESTABILE** is in her fifth year with the Chemistry Department. In her role as the Undergraduate Program Coordinator. she serves as a member of the Chemistry Undergraduate Studies Committee, helping students declare major/minor, their process transfer credit, plan their program of study, track their progress, and coordinates various



undergraduate meetings and events. Deb also enjoys working with faculty and staff to update the department's website, and various printed materials including the departmental newsletter, posters, and brochures. This past year she set up a new Facebook Page for the department (www.facebook. com/UofRChemistry). In add-ition, she is CLASP certified, and assists with the preparation and submission of grant



and fellowship proposals. Deb and her husband celebrated their 25th anniversary in Oct. 2015, and they keep busy with their two boys, ages 14 & 19, and their many activities - including cross country/track, cello concerts, and more. "There's never a dull moment!"

**ROBIN COOLEY** continues to serve as our graduate studies coordinator. She coordinates the recruitment and admission of new graduate students, as well as assisting current students as they progress through their studies toward the doctoral degree. Each year, Robin organizes the department's main recruitment activity, Visitation Weekend, which always draws many prospective graduate students to Rochester. This past year the attendees were welcomed with a star show at the Strasenburgh Planetarium, followed by a full day of activities including tours, faculty talks and dinner at Artisan Works of Rochester. Each fall, Robin also helps organize a week long orientation event for all incoming graduate students. This is a busy week designed to get all of the newest graduate students informed and ready for the start of the new school year. For the 2016-2017 school year, 20 new graduate students were welcomed into the department.



**DONNA J. DOLAN** is currently beginning her twenty-ninth year in Chemistry serving as departmental receptionist and purchaser. In this role, Donna continues to provide support for purchasing in the Chemistry Business Office while also providing assistance to faculty and managing the chemistry department's main office. In

addition, she organizes the departmental distinguished lecturer's program. She has a beautiful addition to her family, great granddaughter Weslynn Althea Watt, born April 9th, 2016. Donna continues to enjoy riding her XL883 Harley.

**GINA EAGAN** is the administrative assistant to Professor Lewis Rothberg, chair of the Materials Science program. With the addition of five Ph.D. and 11 M.S. students this fall, there are a total of 22 Ph.D. and 19 M.S. students in the program. Some of Gina's responsibilities include explaining the graduate requirements to students and faculty, assisting with course registration and exam scheduling, and working closely with the Graduate Studies office and ISO to submit all of the required documentation.

Gina and her kids braved the cold April weather to attend a presidential rally in support of their 6th grade social studies discussions.



#### LYNDA W. MCGARRY (M.S.

**'85)**, completing her sixth year with the department and finishing up her third year as the Development and Alumni Relations Administrator, enjoys working with faculty on preparing grants and awards submissions, as well as organizing alumni and department events. She is also responsible for the annual newsletter. Lynda, her husband Dan, and their family like to get



away to their cottage on Port Bay, a few miles east of Sodus Bay, as often as possible. They enjoy going on the jetski and boat in the summer and snowmobiling in the winter (if we get enough snow!) They also became Buffalo Bills season ticket holders last year, and have enjoyed the tailgating parties with their fellow long-suffering Bills fans.

**KENNETH SIMOLO (PH.D. '85)** starts his twenty-ninth year of service to the University of Rochester. Ken has been assistant chair for administration in the Department of Chemistry since 1988. As assistant chair, Ken manages and advances the administrative and financial functions of the department and also serves as the chief safety officer, helping to ensure that chemistry complies with all EPA and OSHA safety regulations.

**BARBARA SNAITH** began her fifth year with us on July 1st as Administrative Assistant to the Chair of the Department. Barb continues to be a great asset to our Department and enjoys her many responsibilities, including organizing faculty recruiting, attending monthly faculty meetings and preparing the meeting minutes. She also organizes annual staff outings, special events and holiday lunches for the



department. Barb also manages the immigration paperwork needed for the Department's incoming Research Postdoctoral Associates as well 25 visiting students and professors, many of whom are foreign nationals. In her spare time, Barb enjoys fundraising for Lollypop Farm and recently became a Board member for Pet Pride of NY where she helps fundraise for them

as well. In addition, she also supports organizations such as the American Cancer Society (participating in the Breast Cancer Walk every year), Natalie's Wings (organization that supports people with paralysis) and the Upstate Multiple Sclerosis ("MS") Society. She continues to attend GEVA theater productions and Rochester Broadway Theatre League plays with her good friends. Barb is also a captain of a volleyball team that has been playing for years and continues to be active by attending several jazzercise classes every week! She is still a very active member of her church, chairing fundraisers and women's events. Barb has two adorable kitties, Lily and Annabelle, that were 1 year old in September 2016 and continue to entertain her everyday!

**MARGUERITE WESTON** has been with the Department of Chemistry since 1996. She assists faculty by coordinating Chemistry's seminar program with scheduling rooms, contacting speakers to ensure their travel arrangements are in place, obtaining their titles and abstracts, preparing the speakers' schedules of visits with department faculty, along with producing and advertising the online seminar schedule each month throughout the University community. Marguerite also coordinates select special events, assists with various projects, and provides support to numerous faculty members. She coordinates the many administrative details of the annual summer Research Experience for Undergraduates Program (REU). This summer Chemistry's REU program joined forces with its international program that sponsors undergraduates from 6 other countries to do research in the U.S. Marguerite and husband, Art, are residents of Henrietta, NY, enjoy dancing and gardening and have 3 sons and six grandchildren, the newest grandchild being 6 months old. Marguerite retired in January 2017, and we will miss her warm smile, colorful outfits and attention to detail.



# THE EDITORIAL OFFICES

**VALERIE DRAKE** has been working for the past three years with Prof. Kara L. Bren as Editorial Assistant with the *Journal of the American Chemical Society* (JACS). Val and her husband, Lee, are both avid gamers and love tabletop, role-playing, and computer games. Their son, Calvin, is a video game developer with local company Workinman. The photo shows Val with her husband and mother, about to go on a helicopter tour of Maui.



**VALERIE FITZHUGH** continues to enjoy her position as Editorial Assistant for the 16th year, especially the years that she has worked with Prof. Bill Jones at JACS. She likes to tend her garden, but cut back a little this year so that she could spend more time with her grandson Nate who lives with his parents in Chicago, and her sister who arrived from the Cotswolds in England. Val hopes to visit her family in England next summer. Val also enjoys hanging out with her grandsons Rowan and Clark and watching them play hockey. This is a picture of them on their first day of school at McQuaid.



**TERRELL SAMORISKI** began her twelfth year working for *The Journal of Organic Chemistry* (JOC) in August, 2016. Since completing her Ph.D. requirements she has been working remotely with the JOC Chief-Editorial-Office in Salt Lake City, Utah as an Assistant Research Data Analyst. Her first introduction to scientific publication was as a structure editor for the Chemical Abstract Service in Ohio, which she was able to visit in her new role. Terrell left the university in December 2016 to pursue other career opportunities and spend time with her family. We will miss her smiling face!

# **SCIENTIFIC & TECHNICAL STAFF**

**BILL BRENNESSEL** continues to manage the X-ray Crystallographic and CENTC Elemental Analysis facilities. Last November the X-ray Crystallographic and Elemental Analysis facilities relocated to B04 Hutchison as part of a multi-room renovation project. The new room is quite spacious and was engineered to offer optimal climate control for the specific instrumentation. Bill was thrilled to have students from his CHM 417 graduate course in X-ray crystallography, as well as students taking advanced laboratory techniques course CHM 234, work in the new space. According to Bill the new space easily accommodates large groups of people, which is ideal for everything from teaching to hosting tours to conducting meetings, and reaffirms the department's commitment to excellence in teaching and instrumentation support. Bill continues to provides exceptional service year-round to the department's research groups through the techniques of single crystal X-ray diffraction and CHN microanalysis.

Congratulations to **SUSAN CARDINAL**, who was this year's recipient of the **Sandra M. Beach Memorial Award** for outstanding service to the Chemistry Department. Sue began working for the Carlson Science & Engineering Library sixteen years ago, after graduating from Syracuse University's School of



Information. Since then, she has been our "house librarian", helping our faculty and students with tasks from researching chemistry problems, to tracking down books and journals, to doing Internet searches. Whether participating in Chemistry Departmental events, or assisting with faculty and student recruiting, she does so with an enthusiasm for helping that is very unique and infectious. Sue is also responsible for the Chemistry Guide, a valuable resource that is much like Sue herself - a wealth of information. In short, we consider Sue an essential part of the staff that supports Chemistry. Her ongoing efforts certainly make everyone's lives in the Department better, and for that she is well deserving of the award.

The Sandra M. Beach Memorial Award was established as a tribute to Sandra Beach, who served as the Department Secretary from 1991 until her tragic death in an automobile accident in 1993. She was an extremely important and wellliked staff member whose cheerful and helpful attitude made her an invaluable asset. Each year, co-workers, faculty and students nominate a Chemistry staff member whom they feel has contributed significantly to the welfare and camaraderie of the Department.

**JOSEPH HICKEY** is a recent hire for the university. He does safety inspections for the research labs and works with Elly York to prep the undergraduate labs.



**JALIL SHOJAIE** is currently a Sr. lab engineer/chemist who works mornings in the chemistry department and afternoons at the University Laboratory for Laser Energetics (LLE). He has been at the University of Rochester since

1996. He worked as a research chemist in both the obgyn and anesthesiology departments. Prior to coming to Rochester, he worked as a research chemist at NYU, Nelson Institute of Environmental Medicine (1990-95). He has peer-reviewed research publications and patents, with both the University of Rochester and NYU.



**ELLY YORK**, who joined the chemistry department in November of 2006, works part-time prepping for the undergraduate general chemistry laboratories. Elly also assists part-time in the chemistry stockroom. Elly is a graduate of Alfred University and has a Master's degree in education. She also has clinical experience, having previously worked in several veterinary clinics prior to coming to the UR. This year is her tenth year with the department. This summer Elly and her husband and two sons enjoyed visiting family in Florida. This picture was taken in Melbourne, Florida.



# THE BUSINESS OFFICE

The Business Office continues to provide service to faculty, staff and students on all financial matters such as payroll, reimbursements, purchases, preparation of grant budgets and monitoring grant expenditures. **DORIS WHEELER**, business office manager since 2002, is very happy to report that the business office is running smoothly.

**LINDA BOYLE**, a former employee, was recently hired to assist with the day to day accounting responsibiliities. She comes with valuable experience and worked in our department over 20 years ago doing graduate recruiting. She and her husband moved back from New Hampshire to the Rochester area in June.



Anna Kuitems and family

**ANNA KUITEMS** is responsible for reconciling grant ledgers, P-card management and graduate student payroll. **RANDI SHAW** had her 26th anniversary with the University this year. She is the Chemistry Accounting bookkeeper and is responsible for billing internal charges, purchase

orders, reconciling ledgers, employee reimbursement forms, and processing invoices.

**DIANE VISIKO**, TAR accounting bookkeeper, continues to work with departmental payroll and is the 'Timekeeper' for HRMS. With her flexible schedule, she is able to spend more time with her ping sound hild

time with her nine grandchildren.



Diane's Grandchildren

**PAUL LIBERATORE** continues to provide service as the manager of the chemistry stockroom located in the basement of Hutchison Hall. Paul has been with us for 31 years now.

# Instrumentation

The Chemistry Department at the University of Rochester provides a stimulating work environment and is equipped with a wide variety of sophisticated research instrumentation for spectroscopy, analysis, and computation. All of the departmental instruments are used by students and faculty in a "hands-on" manner; most are available 24 hours a day. The opportunities for student use of major state-of-the-art instrumentation represent one of the special strengths of Chemistry at Rochester. The Department acquires the most up-to-date equipment through instrumentation grants from the National Science Foundation, the National Institutes of Health, and other donors. Many of the Department's instruments are highly specialized and in some cases unique, designed and built on site or substantially modified from commercially available instruments to meet the specific needs of the Department's researchers. Staff members are available to train new users, help with troubleshooting, and offer advice on special problems, but the actual measurements are carried out by the individual researchers and the students they mentor. Students learn the theory and practice of a broad range of instrumental techniques in the course of carrying out their research. Several groups in the Department collaborate with scientists and students at the Laboratory for Laser Energetics, an interdisciplinary facility on the University of Rochester campus which conducts cutting-edge research in ultrafast optics and electronics as well as laser fusion.

# **NMR Spectrometers:**

- ~ Varian 500 MHz Inova NMR Spectrometer
- ~ Brüker 500 MHz Avance NMR Spectrometer
- ~ Two Brüker 400 MHz Avance NMR Spectrometers
- ~ Brüker AMX 300 MHz NMR Spectrometer

# **Mass Spectrometers:**

- ~ Thermo Scientific LTQ Velos with Accela LC system
- ~ Brüker Autoflex III Smartbeam MALDI-TOF
- ~ Two Shimadzu GC/MS QP-2010 with EI,CI,-CI
- ~ Shimadzu LC/MS QP-2010, with APCI & ESI

# X-Ray Diffractometers:

- ~ A Siemens SMART CCD X-ray diffractometer with a SMART APEX CCD area detector
- ~ A KRYO-FLEX low temperature device.

# **Photochemistry Facilities:**

- Radiant Dyes RD-EXC-200 excimer laser and Radiant Dyes NarrowScan dye laser for nanosecond transient absorption experiments.
- Continuum high energy picosecond Nd:YAG laser (Leopard, model D-20).
- ~ Tunable, femtosecond Ti : Sapphire laser with harmonic

generator (second and third), and pulse selector coupled to a PicoQuant FluoTime 200 spectrometer and PicoHarp 300 time-correlated single photon counting module.

- ~ Time-resolved, single molecule fluorescence facility, included are: Femtosecond/Picosecond Ti:sapphire
- Oscillator and Optical Parametric oscillator; 2 Avalanche Photodiodes (PicoQuant); Inverted optical microscope (Nikon TE 2000).
- JY Horiba FL3-22 Fluorolog 3 spectrofluorometer equipped with double-grating excitation and emission monochromators.
- Perkin-Elmer Lambda 35 UV-vis-NIR spectrophotometer with a spectral range of 190-1100 pm





Neidig Group member Jared Kneebone inserting his sample into the NMR



PhD student Hanan Alwaseem, in the lab of Rudi Fasan, associate professor of chemistry, demonstrates how she produces analogs of a new compound the lab has developed as a potential treatment for acute myeloid leukemia. (University photo / Bob Marcotte)

# **Other Instruments Include:**

- Shimadzu Model 8400-S Fourier Transform IR configured with a Pike MIRacle ATR sampling accessory - diamond window for analysis of solids, liquids, pastes, and gels.
- ~ Five Shimadzu FTIR Spectrometers
- ~ Remspec ReactionView IR spectrometer with ATR and transmission probes for in situ reaction monitoring.
- ~ Brüker ESP-300 ESR spectrometer.
- $\sim\,$  See Co. MS4 Mössbauer spectrometer equipped with a Janis SVT-400  $\rm L_{_{N2}}/L_{_{\rm He}}$  cryostat
- Magnetic Circular Dichoism spectrometer with a spectral range of 190-2000 nm and temperature control from 1.6 K - 300 K.
- Three potentiostats for electrochemistry from CH instruments
- ~ CENTC Elemental Analysis Facility at the University of Rochester (can handle even water- and oxygensensitive samples)
- Brüker EMX-Plus EPR spectrometer with 4 K temperature Capability

- ~ CEM Explorer Microwave Synthesizer
- ~ Thales Nano H-Cube continuous-flow hydrogenation reactor
- Perkin Elmer 2400 CHN/S Analyzer with VAC Atmospheres (Argon) glove box
- ~ Perkin Elmer Lambda 950 UV/VIS Spectrometer
- Perkin Elmer Lambda 950 UV/VIS Spectrometer with Peltier temperature control unit
- ~ Shimadzu 6300 Atomic Absorption Spectrometer
- ~ Single-molecule time-resolved fluorescence confocal microscope
- ~ Thermogravimetric analysis and Differential Scanning Calorimetry for polymer characterization
- Digital Instruments Nanoscope IIa Atomic Force Microscope
- ~ Ellipsometer
- Spectrofluorometer from Roper Scientific, infared and visible
- ~ Many UV-Vis spectrometers
- ~ Phosphoimager

# **Departmental Funds**

You may also donate online at: http://www.sas.rochester.edu/chm/about/giving.html

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.

## I wish to contribute to the following fund:

Chemistry Alumni Research Fund
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# Esther M. Conwell Graduate Fellowship

This new fund was created in memory of Esther's many accomplishments to the Department of Chemistry and to science more broadly. It will provide support for meritbased fellowships for graduate students pursing a Ph.D in Chemistry who show exceptional promise as researchers. A matching gift component to this fund also exists, whereby any contributions will be matched up to \$20,000 in a calendar year for any gift that is designated to the Conwell Fund. Having fellowships for students provides them the important ability to pursue high-risk/high-reward research not necessarily directly connected to a specific federal grant.

## **Chemistry Department Award for Excellence** in Graduate Education

An anonymous donor has created a new endowed fund to support the awarding of a graduate prize for senior Ph.D. students in Chemistry. The recipient(s) of the prize will be recognized for innovation, industriousness, and creativity in research, teaching and service. The intent is to reward not only students who are successful researchers, but also those who give back to the larger Chemistry community at Rochester through their teaching and service. The prize awardees are expected to be model examples of success for younger graduate students.

Other - Please specify My gift is in honor of		(see above)
act Information:	Degree Informa	ition:
ME	Year degree(s) received	l from the Department
FSS	B.A	M.S
	— B.S	PH.D
	ADVISOR	

Please send your contribution and this form to: Development Administrator, Department of Chemistry, University of Rochester, RC Box 270216, Rochester, NY 14627-0216.

# Alumni Update

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

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

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	University of Rochester Department of Chemistry RC Box 270216 Rochester, New York 14627-0216	585-275-2915 (phone) 585-276-0205 (fax) email: alumni@chem.rochester.edu www.sas.rochester.edu/chm/alumni/
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