

A photograph of a modern, multi-story brick and concrete building, likely a chemistry department building at the University of Rochester. The building features a prominent concrete staircase on the left side and several balconies with brick railings. The sky is clear and blue.

University of Rochester
CHEMISTRY

ANNUAL NEWSLETTER
2012-2013

EASTMAN
QUADRANGLE



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Greetings to all Department of Chemistry Alumni!

We enjoyed a busy and productive 2012-2013 year in the department and at the University. As I complete my tenth and final year as chair of the Department of Chemistry, I am happy to share with you some of the developments within the department and University from the past year.

The economic stress that the US has been experiencing since 2008 continues to have an impact on the University and to a lesser extent the department. The University has made sustaining the quality and distinction of our undergraduate programs one of its highest priorities and is devoting a considerable proportion of available resources to help students and their families weather the continuing difficult economic times with respect to achieving a college education. The primary impact on the department has been seen in a somewhat restrained rate of growth of the faculty.

Four types of financial support drive our academic programs: tuition, sponsored research, gifts, and endowment distribution. The University Endowment has largely recovered from the events of 2008, but the College's (including the Schools of Arts & Sciences, and Engineering & Applied Sciences) draw on their portion of the unrestricted endowment had been historically too high for overall fiscal prudence and has been scaled back to a sustainable level near ~5.5%. Most of the UR's academic divisions in The College of Arts, Sciences, and Engineering, including the chemistry department, are tuition driven. The very good news is that we experienced another record year of applications to the undergraduate program at the College and the ten year growth plan is on track. We have over 5100 matriculated undergraduate students for 2013-2014. Since the chemistry department anticipates that a proportionate number of incoming freshmen will participate in the chemistry

curriculum, to sustain the growth in enrollment and maintain acceptable class sizes, we need to grow our tenure-track faculty. We have added one new tenure-track faculty member, Ignacio Franco, a theoretical physical chemist, this July 2013. Regrettably, we have had one departure as Patrick Holland accepted a position at Yale University.

New research initiatives, such as those in systems biology, nanotechnology, renewable energy (particularly fuel cell and hydrogen production), big data science, and identification of gene function, are clearly areas of critical importance to the nation. As a central science, chemistry has an essential part to play in the nation's research enterprise. Despite the potential impact of the sequester and projected decrease in Federal research support, the department increased its sponsored research expenditures to \$6.0M in 2012. UR chemistry faculty have successfully applied, and will continue to apply, for federal funding as well as other state and foundation programs. Last year our faculty received both new and renewed funding for their various research programs from agencies such as the DOE, NIH, and NSF; junior faculty were successful in competing for funding from the ACS, NIH, NSF, and the Provost's Multidisciplinary Research Award as well as others. However, given the fiscal stress which the federal government is experiencing and the obvious need to reduce federal deficits, the future of government supported science research is cloudy. Science research is funded out of the discretionary portion of the federal budget and likely to come under unprecedented pressure in the coming few years as entitlement and other mandated programs take up a larger and larger portion of taxes and other revenue. The percentage of NIH and NSF grant applications funded are already at or near historic lows; the coming years are going to present enormous challenges for academic science to find ways to fund their programs with fewer federal research dollars. This translates to greater reliance on foundations, other private sector support, and alumni. We are pleased to see that our loyal UR chemistry alumni have continued their strong, generous support of the department through contributions to the Alumni Research Fund.

Several chemistry faculty received notable awards this year. Todd Krauss was named a Fellow of the American Physical Society, Richard Eisenberg received both the Fred Basolo Medal and the ACS William H. Nichols Medal, and Dan Weix received an Alfred P. Sloan Fellowship and Thieme Chemistry Journal Award. In addition, two of our faculty received teaching awards: Alison Frontier the 2012 Goergen Award for Distinguished Achievement and Artistry in Undergraduate Teaching and Ben Hafensteiner the UR Professor of the Year in Natural Sciences. These kinds of recognitions help to sustain our efforts to recruit and retain high quality faculty and students, and enhance the reputation of the department and the University. Faculty innovation in research, coupled with excellence in teaching, comprise the core of our Ph.D. program, providing a rich environment for student knowledge

and research that is fundamental to science education in the 21st century. Chemistry students, too, received a large number of awards, opportunities, and fellowships last year, including one international NSF Graduate Research Fellowship Award and two NSF GRF Honorable Mentions. Katherine Garner, B.A. '11/T5 '12, received a Carnegie Junior Fellowship, the first ever for the University of Rochester. Efforts to remain on the cutting-edge of research and education are ongoing, as you will read about in the rest of the newsletter.

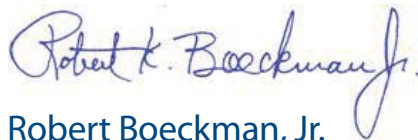
The University is more than halfway through a major gift campaign to help raise funds for new endowed professorships and needed infrastructure improvements, including new or renovated buildings for science. Through the generous gifts of our alumni and other university and unrestricted funds, we will continue the staged renovation of chemistry's research laboratories over the next several years. We are hopeful that funds will also become available to continue the urgently needed upgrades to our teaching laboratories and to the infrastructure of Hutchison Hall. Hutchison Hall is now 40 years of age, and is showing the wear and tear of its 40 years of fine service. Owing to increasingly stringent environmental and safety regulations, major renovations of the central building infrastructure are required that will return what is otherwise a sound and serviceable structure to a modern facility meeting all current and anticipated near-term needs.

Let me close by thanking all of you, both alumni, faculty, staff, and students for your personal support and assistance during my 10 year tenure as Chair of Chemistry. I have been gratified by the progress we made during this time, and I am most grateful to the faculty and staff of the Chemistry Department for making my term as Chair so personally rewarding. I can honestly say that the Department is a wonderful place to work and that I work with a truly remarkable group of people. I will be ably followed by Todd D. Krauss as Chair. Todd is a vigorous young leader who will take the Chemistry Department to new heights. Please welcome him and accord him the same strong support in the coming years.

I am also extremely grateful to our alumni for your continuing support of the Department over the years. The support and advice of our alumni is an invaluable resource. We continuously endeavor to establish and nurture our collegial atmosphere and sense of community with our alumni. We are happy to receive news and are proud of your achievements in your respective fields. Please let us know how you are doing by using the reply form at the back of this newsletter or online at <http://www.chem.rochester.edu/alumni/submitnews.php> and we will pass the word on in next year's edition. We encourage you to stay in touch through the newsletter, through attending events, and through our website at www.chem.rochester.edu. We want our current students to appreciate the legacy of our extended "Chemistry Family" through a bond with their predecessors.

Meliora and thank-you! Best wishes to all for a successful and happy year in 2013-2014.

Sincerely,



Robert Boeckman, Jr.



The faculty, staff, and students celebrated Bob's ten years with an afternoon get together in the Green Carpet Lounge on Friday, June 21, 2013. Everyone enjoyed the fun, friendship and food culminating in giving Bob his very own "Bob"blehead!

This was followed by a dinner at the beautiful Woodcliff Hotel and Spa on Monday night, June 24th, where Bob and his wife, Mary, enjoyed a dinner with faculty and friends. Bob was toasted and lightly "roasted" by Todd Krauss, Rich Eisenberg, and Pat Holland.

Mary and Bob Boeckman



**THANK YOU
BOB!**

We appreciate all
your hard work and
dedicated service
as Chair for the past
ten years.

Meet the New Chair



Greetings to all Chemistry Department students, faculty, staff and especially our alumni!

The Chemistry Department at Rochester is entering a year of transition as after 10 years as Chair, Bob Boeckman has returned to the “ordinary” faculty life of teaching and research. The Department has had much positive change under Bob’s leadership and I list a few examples here:

- The number of undergraduate Chemistry majors has grown by 175 % to a total of 50 in the last year.
- The graduate program has grown significantly as well from 72 students in 2003 to a total of 120 students today.
- A cohort of talented young faculty have matured and are poised to lead their fields, leaving the Department with the lowest percentage of untenured faculty in over two decades.

On behalf of the entire Chemistry Department we want to thank Bob for 10 years of selfless service and offer hearty congratulations on a job well done. As I begin my term as Chair I already have a deep appreciation for the challenges of this position, and hope that I will be able to continue the momentum that Bob has brought to the Department this last decade.

We want to extend a warm welcome into the Department to Ignacio Franco, who started as an Assistant Professor in July of 2013. Ignacio is a theoretical chemist who will work on the behavior of molecules under mechanical, optical or electrical stress. He received his Ph.D. in Theoretical Chemical Physics from the University of Toronto Canada, after which he

joined Northwestern as a postdoctoral fellow, and then took a position as group leader and Humboldt research fellow in the Theory Department of the Fritz Haber Institute in 2011. We expect that going forward Ignacio, along with Oleg Prezhdo, will form the basis of a strong core theoretical group in the Department.

As we look ahead to the academic year 2013-2014 I wanted to share some of the goals and objectives of the Department. In the last five years or so University has seen a 20% increase in undergraduate enrollment bringing the total matriculated undergraduate students to over 5100. What has not kept pace with the growth in the University as a whole is the growth in the number of tenure-track Chemistry faculty. As a result, Chemistry faculty are teaching well over 25% more students than 10 years ago, yet the number of tenure-track faculty has not increased even by one. Further, as the field of Chemistry diversifies into a rich set of interdisciplinary areas, we have been struggling to keep up due to the constrained size. Thus, one of our critical goals as a Department is to obtain the resources, both internal and external to the University, such that we can reach a faculty size of 25 within 6 years by hiring at least 10 new faculty over that time period. In addition to strengthening the core areas of physical, inorganic and organic chemistry with our hires, we look to build on our strengths in emerging areas of chemistry such as chemical biology, supramolecular systems, materials, and nanoscience/nanotechnology. This hiring plan is an ambitious goal and we look forward to working with all the stakeholders to ensure that it comes to fruition. Having a larger faculty size will allow Chemistry at Rochester to remain competitive with our peer institutions and allow us to recruit to Rochester the best and brightest faculty and students.

Where possible, our current and future research activities will be focused on three “grand challenges” facing society today that can be directly and significantly impacted by chemistry: (1) Energy: meeting global energy needs while responsibly maintaining environmental resources; (2) Sustainability: meeting the needs of a growing worldwide population given limited global resources; and (3) Human Health: enhancing global human health through disease prevention and treatment and by enabling a healthy lifestyle. As the “central science,” Chemistry is uniquely positioned to address these three challenges through interdisciplinary research initiatives. Indeed, already this year two major proposal efforts have been submitted to the National Science Foundation to support Centers of Excellence around the areas of “sustainable catalysis,” “topologically switchable soft materials,” and “multifunctional carbon-based membranes.”

We are looking to also broaden our undergraduate course offerings to include several “fun” classes (not that sophomore Organic chemistry was not fun). Already being offered is a

course on Energy Science, Energy Technology and Energy in Society being taught by Udo Schröder, which aims to give students a scientific-technological knowledge base concerning conventional and novel energy production and distribution technologies such that they can critically evaluate existing and proposed energy policy scenarios. In development is a course by Alison Frontier on the chemistry and biochemistry of poisons, and the relationship of these poisons to both recreational drugs and pharmaceuticals. Over the longer term, I would like to develop a course on the Art and Science of Cooking. Challenges remain as to their eventual adoption, such as how does one teach a cooking course laboratory in Hutchison Hall, but nonetheless we look forward to moving ahead quickly and expect these courses to be quite popular once offered.

Finally, I look forward to engaging our chemistry alumni around the country over the coming years in a discussion of how to best advance Chemistry at Rochester. These conversations take on additional importance as we enter what seems like an era of ever decreasing federal resources and serious questions at all levels of government about the costs of a higher edu-

cation and whether an institution such as Rochester provides a reasonable “value” to the student. To that end I wish to extend a personal invitation to return to Rochester for Meliora Weekend, with events running October 10th through the 13th. In particular, please note that this year we will have the annual Chemistry Department Gates Happy Hour on campus in the Susan B. Anthony Residence Hall’s Friel Lounge on Saturday, October 12th, from 4:30 to 6:00 pm. The Gates Happy Hour is hosted by Ginny and Rob Searl, family of the late Professor and Chair, Marshall D. Gates, Jr. I look forward to meeting you there!

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

Sincerely,



Todd D. Krauss

Todd D. Krauss Elected APS Fellow

Todd D. Krauss, professor of chemistry and optics, has been elected a Fellow of the American Physical Society (APS) in recognition for outstanding contributions to the field of nanoscience, especially the photophysics of nanoscale semiconductors, including groundbreaking discoveries of the fluorescence properties of single carbon nanotubes and individual semiconductor nanocrystals. Todd’s postdoctoral advisor, Louis Brus of Columbia University, commented that Todd “has a sense for putting things and people together from available resources, so that significant research gets done. Krauss has become a major member of the US nano-science community. . . . and his work is quite novel. He will be productive for many years to come.”

Todd and his group have established an innovative and interdisciplinary research program focusing on understanding the fundamental optical properties of nanomaterials and integrating them into new technologies for biology, optics and electronics. More than of interest to specialists, their research has tried to address challenging problems that capture the attention of generalists, and that also has ramifications across several fields. Specifically, they have distinguished themselves in three distinct areas of nanomaterials science: carbon nanotube

photophysics, semiconductor nanocrystal photophysics, and semiconductor nanocrystal synthetic mechanisms. Altogether, Todd’s research is by its very nature highly interdisciplinary, and has made significant impacts in chemistry, applied physics, physics, biophysics, optics and materials science.

Todd was inducted as an APS Fellow during the March, 2013 meeting held in Baltimore, Maryland. In the Chemistry Department, he joins his colleagues, James Farrar, John Huizenga, John Muentner, Oleg Prezhdo, Lewis Rothberg, and Udo Schroeder as Fellows of the APS.

The APS is a non-profit membership organization working to advance and diffuse the knowledge of physics through its outstanding research journals, scientific meetings, education, outreach, advocacy and international activities. APS represents over 50,000 members, including physicists in academia, national laboratories and industry in the United States and throughout the world. Society offices are located in College Park, MD (Headquarters), Ridge, NY, and Washington, DC. The Division of Chemical Physics (DCP) within the APS exists to provide a forum for those who work to understand a broad range of chemical systems, from atomic collisions to complex materials, in terms of the behavior of the individual atoms and particles that make up the system.

Donors '12-'13

Includes donations received between July 2012 and June 2013.

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Pfizer Corporation, Inc.
Roche Labs
Shell Oil Company Foundation
Texas Instrument, Inc.



KATHERINE GARNER (B.A. '11/T5 '12) left for Washington, D.C. this August to participate in the Carnegie Junior Fellows program. She is among ten students and recent college graduates selected to provide research assistance in 2013-14 to senior scholars working on Carnegie Endowment for International Peace (CEIP) programs. The Carnegie Junior Fellowship is a highly selective program that accepts just five percent of its applicant pool. Candidates must be nominated by their college or university, Rochester having joined the list of ~ 400 participating institutions in 2004. Garner is the first candidate to be selected.



“It is a tremendous accomplishment for Kate Garner to have been selected as the first-ever Carnegie Junior Fellowship finalist and winner from Rochester this year,” said Belinda Redden, director of fellowships at Rochester. “Her year at the Endowment will be a transformative experience. Not only will she obtain a keener understanding of the politics of climate change and energy issues, but she will also gain greater insight into how she can best marshal her talents and commitment to science, public policy, and effective public outreach in the realm of environmental challenges and sustainable solutions.”

A native of Cheshire, Conn., Garner will spend one year working under senior associate Deborah Gordon through the Carnegie Energy and Climate Program, researching the policies and regulations surrounding unconventional oils and water usage. It's a subject that has always been of interest to Garner. As an undergraduate, she enrolled in Physical Hydrology, which explored how water is used as a resource for human consumption and touched on governmental regulation of water. This sparked a curiosity in policy for Garner, who said the Carnegie Junior Fellowship will be an opportunity to delve deeper into the subject. She'll assist Gordon in creating a database that tracks the total carbon footprint of unconventional oils. Pending funding, she also may research how states currently regulate water usage, as a way to benchmark the best way to regulate water use for producing unconventional oils.

Two University of Rochester students and eight alumni have been named recipients of the National Science Foundation Graduate Research Fellowships. Additionally, 13 current students and recent alumni were given honorable mentions by the NSF. The fellowship, which is part of a federally sponsored program, provides up to three years of graduate study support for students pursuing doctoral or research-based master's degrees. Since the program's inception in 1952, it has supported nearly 50,000 students conducting research in science, technology, engineering, mathematics, and selected social science disciplines. Of the more than 12,000 applicants, only 2,000 were awarded fellowships. The fellowship includes a three-year annual stipend of \$30,000, a \$12,000 educational allowance to the institution, and international research and professional development opportunities. Two chemistry alums received Honorable Mention - **MATTHEW D. DEMARS II (B.A. '12 - Fasan/B.S. '12 BIOCHEMISTRY)** a graduate student in chemistry at the University of Michigan, and **JONATHAN M. GOLDBERG B.S. '12** - Holland) now a graduate student in chemistry at the University of Washington.

JENNIFER CIESIELSKI (PH.D. '12), from Alison Frontier's group, defended her Ph.D. thesis last summer and was awarded a National Science Foundation (NSF) International Research Fellowship. The objective of the International Research Fellowship Program (IRFP) is to introduce scientists and engineers in the early stages of their careers to international collaborative research opportunities, thereby furthering their research capacity and global perspective and forging long-term relationships with scientists, technologists and engineers abroad. These awards are available in any field of science and engineering research and education supported by NSF.



Jennifer is working at the ETH (Swiss Federal Institute of Technology) in Zurich, Switzerland for Professor Erick M. Carreira. Prof. Carreira's research is focused on synthetic organic chemistry, organometallics and asymmetric catalysis, and medicinal chemistry.

TRAVIS J. HEBDEN (B.S. '04, M.S. '05) and his wife, Michelle Cataldo Hebden, welcomed their second daughter, Isadora, earlier in 2012. Travis, who received his Ph.D. in Chemistry under D. Michael Heinekey at the University of Washington in 2009, finished his postdoc at MIT and is now working for Portland Technology Development group's Thin Films division of Intel in Hillsboro, Oregon. PTD Module Engineers are responsible for leading scientific research and enabling manufacture of innovative device architectures coupled with the realization of these architectures.



KAREN CHIANG (PH.D. '12) moved to San Diego last year after defending her thesis to join her then fiance, now husband, **ABDALLAH BITAR (M.D./PH.D. '09)**. Dr. Bitar is a resident in the physician-scientist track of Scripps Clinic's Internal Medicine Residency Program and recently joined as a KL2 Scholar at STSI. Dr. Bitar has a passion for drug development and design, hoping to continue this line of work with the Scripps Translational Science Institute.



Karen is now a part-time post-doctoral researcher and undergraduate mentor at the University of San Diego with Professor Timothy Clark. The Clark research group focuses on the applications of organometallic chemistry to organic synthesis.

Karen has a special interest in becoming involved with organizations that share the mission to promote understanding of the sciences in youths and adults. She mentions that her time in graduate school (Pat Holland's group) made her realize that there is a large need for communicating science to the general public by using fun and interactive methods to make science more palatable.

On October 23, 2012, **Norman P. Neureiter (B.A. '52)** was awarded the Austrian Cross of Honor in Science and Art 1st Class, in the name of the President of Austria and presented by the Austrian Minister of Science and Research at a gala dinner event celebrating the 40th Anniversary of

IIASA—an international organization whose mission is to address the major problems facing mankind, such as energy, food, water, population, and climate change.

Dr. Neureiter was born in Illinois and grew up near Rochester, New York. After receiving his B.A. degree in chemistry from the UR, he completed his Ph.D. in organic chemistry from Northwestern University in 1957. He spent a year ('55-6) as a Fulbright Fellow in the Institute of Organic Chemistry at the University of Munich then joined Humble Oil and Refining (now part of Exxon) in Baytown, Texas as a research chemist. On leave from Humble in 1959, he served as a guide at the U.S. National Exhibition in Moscow, subsequently qualifying as an escort interpreter for the Department of State. Thus began many years in government service both here and abroad. He left government service in 1973 and joined Texas Instruments (TI), where he held a number of staff and management positions.



Minister Töchterle (left) awarding Norman Neureiter the Austrian Cross of Honor for Science and Art 1st Class.ACS

Norman retired from TI in 1996, and worked as a consultant until being appointed as the first Science and Technology Adviser to the U.S. Secretary of State from 2000-2003. He was then made a Distinguished Presidential Fellow for International Affairs at the U.S. National Academy of Sciences (NAS). In 2004, he joined the American Association for the Advancement of Science (AAAS) to become the first Director of the newly established AAAS Center for Science, Technology and Security Policy (CSTSP). Although he stepped down as the Director of CSTSP in 2009, he remains as Senior Advisor both to CSTSP and the recently formed AAAS Center for Science Diplomacy (CSD). Dr. Neureiter is a Fellow of the American Association for the Advancement of Science and in 2008, he was elected a Fellow of the American Academy of Arts and Sciences and also was a recipient of the National Academy of Sciences' Public Welfare Medal, considered the highest honor of that institution. In 2010, he received from the Emperor of Japan the Order of the Rising Sun, Gold and Silver Star, for contributions over many years to furthering scientific cooperation between the U.S. and Japan. He is presently also a member of the NAS Committee on International Security and Arms Control (CISAC). Dr. Neureiter is married with four children and speaks German, Russian, and Polish.

IN MEMORIAM

JOHN K. BORCHARDT (Ph.D. '73), 66, an oil and energy consultant, technical writer, and ACS career consultant, died in January, 2013 while attending an ACS Leadership Institute meeting in Dallas. A native of Chicago, Borchardt earned a B.S. in chemistry from Illinois Institute of Technology in 1968 and a Ph.D. in organic chemistry from the UR in 1973. He worked at Halliburton Services from 1977



until 1984, when he moved to Shell Chemical. In 1999, he moved to Tomah Products, where he served as a technical manager for three years. In 2005, he began working as a technical writer and volunteer career consultant with ACS. He authored the ACS/Oxford University Press book "Career Management for Scientists and Engineers" and authored or coauthored more than 1,500 career-oriented articles published in magazines, newspapers, and encyclopedias.

"John had an enormous impact in the lives of hundreds of students and chemists," says David Harwell, assistant director for career management at ACS. "He devoted himself to service and was a foundational and ever-present volunteer," he adds. Indeed, John visited Rochester in the fall of 2010 and presented "Managing Your Job Search" at our annual SYCAM (Synthesis, Catalysis, & Mechanism) cluster retreat. He also held individual meetings with students to review their resumes and give suggestions for interviewing. John is survived by two brothers.

ELLIS R. GLAZIER (Ph.D. '57), 83, passed away in La Paz, Mexico in April, 2013. Born in Allentown, NY, he was the son of the late Harry A. and Clara Glazier. Ellis was a graduate of Allentown High School, Cornell University, and received his doctorate in chemistry from the University of Rochester. He served in the U.S. Army Air Corps during the Korean War. Ellis had been living in Mexico for the last 24 years working in his second career as an author's editor of scientific papers. He stated just this past fall that "it has been a great educational experience, especially in marine science, because La Paz is situated on the Mar de Cortes. Ellis also worked with a group at the Universidad Nacional Autónoma de México (UNAM) and the Universidad de Puebla. He is survived by his wife, Eileen; brother, Leonard; sons, Charles and Jonathon; and five grandchildren.

JAMES G. SMITH (B.S. '53), who passed away in January, 2013 at the age of 84, was a retiree of Eastman Kodak Co., with 42 years of service. Jim also did IRS tax preparation for seniors and was an usher at Eastman Theater for many years. In addition, Jim volunteered with the Monroe County Cooperative Extensive whose mission is to provide research-based information and education programs to address local priority needs in the areas of 4-H Youth Development, Agriculture, Horticulture, and Nutrition, Food Safety & Health. Jim is survived by his wife, Doris, and son, Keith.

The Department of Chemistry also mourns the passing of:

- ☞ Ernest Royal Hanna (Ph.D. '59)
- ☞ Arthur Gene Krohn (B.A. '59)
- ☞ William L. Lehn (Ph.D. '58)
- ☞ Charles A. Manuele (B.A. '35)
- ☞ Robert James Scott (B.S. '48)

Interfaith Chapel (Photo Courtesy of Bruce Benerofe)



Richard Eisenberg Receives William H. Nichols and Fred Basolo Medals

Rich receiving the William H. Nichols Medal from Philip Mark, Chair of the NY Section of the ACS

Congratulations to Rich Eisenberg who was named the 2013 William H. Nichols Medal award winner “for contributions to Inorganic Photochemistry” and the 2012 Fred Basolo Medal Award winner for “outstanding research in Inorganic Chemistry!”

Richard Eisenberg, Tracy Harris Professor of Chemistry, received his undergraduate and graduate degrees from Columbia University. In 1973, he joined the faculty of the University of Rochester after six years as Assistant and Associate Professor at Brown University in Providence, RI. He served as Chair of the UR Chemistry Department from 1991-1994 and was named to the Harris Chair in 1996. Rich served as the Editor-in-Chief of *Inorganic Chemistry*, the leading journal in its field, during the period 2001-2012.

Eisenberg’s research interests are in inorganic and organometallic chemistry, photochemistry relating to solar energy conversion, and catalysis. Some of Eisenberg’s specific research activities include the photogeneration of hydrogen from water, luminescent square planar complexes and their incorporation into molecular assemblies for photoinduced charge separation, the development of parahydrogen induced polarization for hydrogen addition reactions, luminescent gold and copper complexes for application in electroluminescent. He has won numerous awards including the 2003 ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry and shared the 2011 ACS Nobel Laureate Signature Award in Graduate Education with his student Ping-wu Du. In 2010, he received the Lifetime Achievement Award for Graduate Education from the University of Rochester. Eisenberg was elected a Fellow of the American Association for the Advancement of Science in 2005, a Fellow of the American Academy of Arts and Sciences in 2009, and a Member of the U. S. National Academy of Sciences in 2010.

The William H. Nichols Medal Award, the oldest award presented by a local section (New York) of the ACS, recognizes outstanding achievement in chemical research. Dr. William H. Nichols, a charter member of the American Chemical Society and its president in 1918 and 1919, was a pioneer in the development of the chemical industry in the United States and an early champion of the importance of chemistry in the future growth of the



nation. He maintained a deep commitment to research and development and to the importance of supporting science education and students of chemistry. To date, 16 recipients of the Nichols Medal have also received the Nobel Prize. The Nichols Medal was presented to Professor Eisenberg in March of 2013 and was coupled with a symposium in which Harry Gray, Cliff Kubiak, Bill Jones and Marcetta Darensbourg all participated.

The Fred Basolo Medal was established by the former students of Fred Basolo in appreciation for his contributions to inorganic chemistry at Northwestern University. Internationally recognized for his original contributions to the syntheses and reaction mechanisms of transition-metal Werner complexes, Basolo did some of the seminal work in the developing fields of organometallic and bioinorganic chemistry. Fred was a member of the National Academy of Sciences, the American Academy of Arts and Sciences, and received ACS Awards for Research and for Service in Inorganic Chemistry, the Pimentel Award in Chemical Education and the 2001 Priestley Medal.

Rich was presented the Basolo medal in October, 2012 at Northwestern University where he spoke on “The Reductive Side of Water Splitting: Recent Progress in the Photo-driven Generation of Hydrogen from Water.” The Basolo medal was particularly meaningful because Rich is a “scientific grandson” of Fred’s and knew Fred for many years.

Sloan Research Fellow Dan Weix Thieme Chemistry Journal & Pfizer Green Chemistry Awards

We want to congratulate Dan Weix, Assistant Professor of Chemistry, for a great year! He was named a 2013 Sloan Research Fellow, received a 2013 Thieme Chemistry Journal Award **and** a 2012 Green Chemistry Award from the Pfizer-Groton Green Chemistry Team!

Dan Weix has made a tremendous start in his research and teaching career since joining our faculty as a tenure-track faculty assistant professor on July 1, 2008. Dan came to Rochester with an extremely strong background in synthetic and organometallic chemistry, focusing on the development of new methods for C-C bond formation used in organic synthesis. He earned his B.S. in Chemistry at Columbia University in 2000, and his Ph.D. degree under the direction of Professor Jonathan Ellman at the University of California, Berkeley in 2005. He spent three years as a postdoctoral fellow with Professor John Hartwig at Yale University and the University of Illinois at Urbana-Champaign prior to joining our department.

According to Chemistry Chair Robert Boeckman, Jr., “There is no question the breadth and depth of Dan’s research program, developed in a mere four years, ranks him at the very top of his cohort of young faculty working in the area of organometallic synthesis methodology.” Dan notes that it is “a real honor to receive these honors on behalf of my research group. Their hard work and insights have made this possible and enjoyable. These honors, both from academia and industry, reflect the conceptual and practical advances we have been able to make in Cross-Electrophile coupling these past few years.”

The Alfred P. Sloan Foundation is a philanthropic, not-for-profit grantmaking institution based in New York City. Established in 1934 by Alfred Pritchard Sloan Jr., then-President and Chief Executive Officer of the General Motors Corporation, the Sloan Research Fellowships seek to stimulate fundamental research by early-career scientists and scholars of outstanding promise. Nominated by their fellow researchers and chosen by a distinguished panel of senior scholars, the Sloan Research Fellows represent the next generation of leaders in the natural sciences, economics, and mathematics. These two-year fellowships are awarded yearly to 126 researchers in recognition of distinguished performance and a unique potential to make substantial contributions to their field. Past



Dan Weix (left) with undergraduate student David George (B.S. '12 - center), and group member, Dan Everson at the Undergraduate Research Expo, spring 2013

recipients of Sloan Research Fellowships have gone on to win 38 Nobel prizes, 14 Fields Medals (mathematics), and eight John Bates Clark awards (economics).

Dan Weix was also the recipient of a 2013 Thieme Chemistry Journal Award - established in 1999 with the aim to encourage young scientists. This award is granted to prospective chemists who have been recognized as high-potential researchers in the field of synthetic organic chemistry by the editorial board members of *Synthesis*, *Synlett* and *Synfacts*.

Lastly, the Weix group was chosen for a Pfizer Green Chemistry Award. Pfizer Worldwide Research & Development in Groton, Connecticut, actively promotes the twelve principles of green chemistry amongst their staff. One of the key components of the program facilitated by their Green Chemistry Team is internal recognition through the “Groton Labs Green Chemistry Award.” Annual awards are presented to Pfizer scientists who demonstrate outstanding performance by incorporating green chemistry into pharmaceutical research and development activities. As part of the award, the winners of the Groton Green Chemistry Award receive a \$5,000 cash award for a university scientific department selected by the winner(s). The 2012 winners have chosen to donate \$5,000 to the Weix research group in the Department of Chemistry at the University of Rochester to recognize the group’s notable contributions to the increasingly important field of Non-Precious Metal Catalysis.

Harrison Howe Award: Sunney Xie

The 2012 Harrison Howe Award of the Rochester Section of the American Chemical Society was presented to Professor Xiaoliang (Sunney) Xie, on October 2, 2012 during the Northeastern Regional Meeting (NERM) of the ACS held in Rochester at the RiverFront Radisson. The Harrison Howe Award is dedicated to the memory of Harrison E. Howe, 1881—1942, a cofounder of the ACS Rochester Section and a well-known chemist, editor, and author. The award was established to recognize a scientist who has made outstanding contributions to chemistry or closely related fields and who shows great potential for further achievement. There have been 67 Harrison Howe Award winners, twenty-six of



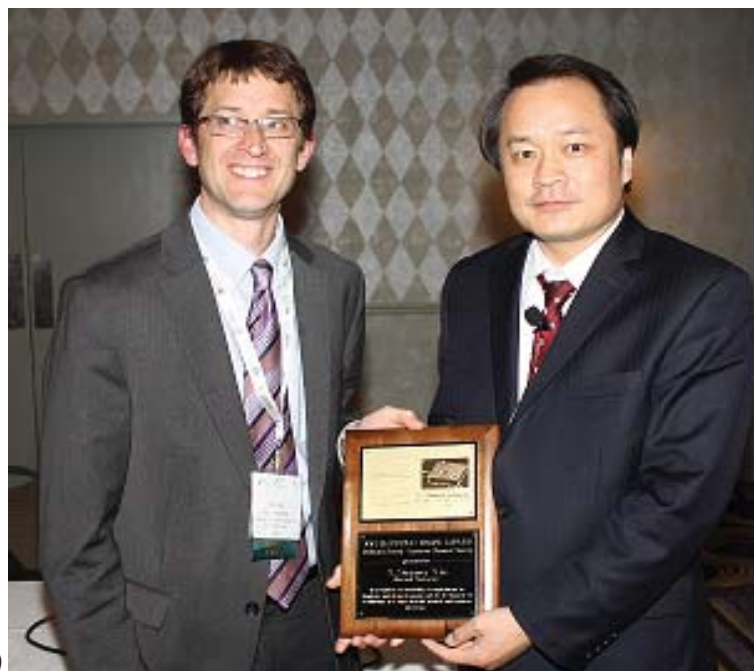
whom subsequently won a Nobel Prize (39%). Professor Brad Nilsson is the current chair of the Harrison Howe Award Committee, which also includes Professors Todd Krauss and David McCamant as committee members.

Sunney Xie, considered a founding father of single-molecule enzymology, received a B.S. from Peking University in 1984, and a Ph.D. from the University of California at San Diego in 1990, followed by a short postdoctoral experience at the University of Chicago. In 1992, Xie joined Pacific Northwest National Laboratory, where he later became a Chief Scientist. In 1999, he was appointed Professor of Chemistry at Harvard University. He is now the Mallinckrodt Professor of Chemistry and Chemical Biology at Harvard.

His honors include the E.O. Lawrence Award in Chemistry, the Leibinger Innovation Prize, the NIH Director's Pioneer Award, and the Sackler Prize for Physical Sciences. Xie is a fellow of the American Academy of Arts and Sciences and a member of the National Academy of Sciences. Xie's group is working at the interface of several disciplines, striving to develop new physical and chemical tools to solve compelling biological problems. Xie has made major contributions to the emergence of the field of single-molecule biophysical chemistry and its application to biology. Recently, they have developed a new DNA sequencing method that offers potentially low cost and fast turnaround time for genome analyses. They are exploring single cell genomics, which allows

the determination of the genome of an individual cell. His team also pioneered the development of coherent Raman scattering microscopy. With a wealth of physical and chemical tools, Xie's group is excited to make both scientific and technological contributions to life science as it is becoming a data-rich, quantitative science.

To celebrate the event, an afternoon symposium, entitled "New Frontiers in Imaging" was organized by Profs. Brad Nilsson and David McCamant. The symposium included a seminar by X. Sunney Xie, entitled "The Quest for Non-linear coherent optical imaging for biology and medicine". This was followed by Prof. Ed Brown, of the University of Rochester Medical Center, who described his work using second-harmonic generation with femtosecond lasers to probe collagen in breast cancer tissue. Two alums, Haw Yang (Princeton) and Peng Chen (Cornell), from the Xie lab were also in attendance. Prof. Haw Yang, from Princeton's Department of Chemistry, discussed his recent microscopy work investigating conformational dynamics of enzymes and temperature gradients in single cells. Prof. Peng Cheng, from Cornell's Department of Chemistry, spoke about his single particle studies of catalysis by metallic nanoparticles. The evening award ceremony began with a delightful reception overlooking the Genesee river and dinner, followed by the award ceremony and public lecture by Prof. Xie, in which Prof. Xie described his work investigating single molecule enzymology and imaging. Attendance at the public lecture was estimated at over 200.



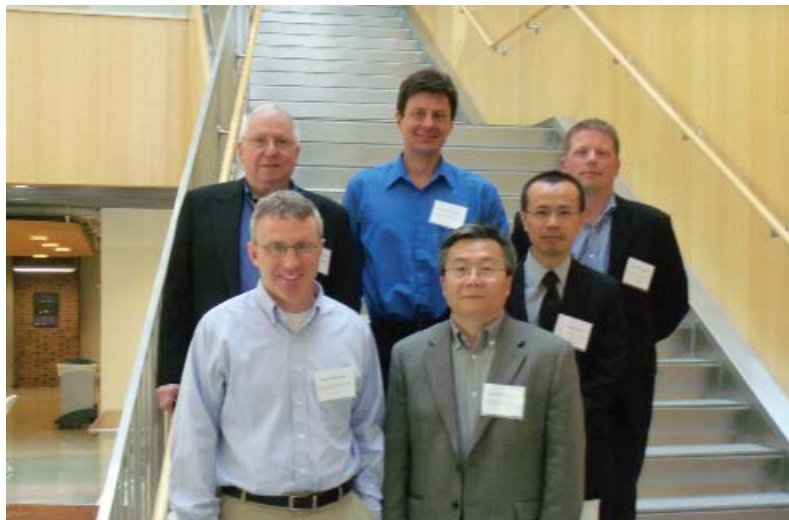
Dave McCamant and Sunney Xie (right)

Nanomaterials Symposium 2013

On Monday, May 20, 2013, the Rochester Advanced Material Program (RAMP) hosted the Nanomaterials Symposium 2013 on Frontiers in Materials Science for the 21st Century: Novel Materials for Sustainable Catalysis. This event was co-sponsored by the Hajim School of Engineering & Applied Sciences, the School of Arts & Sciences and the UR Integrated Nanosystems Center. The symposium committee faculty members were Professors Todd Krauss and Oleg Prezhdo. The event coordinator was Lynda McGarry, with special thanks to Breanna Eng ('13) for the design and publication of the symposium web page and program brochure.

One of the great synthetic challenges for the 21st century is the design of materials and chemical fuels of all types utilizing sustainable and/or green processes. The one-day “Gordon conference” style symposium had an overarching theme of innovation in materials science and engineering that will be necessary in order to advance catalytic applications in the coming decades. Keynote speakers addressed the problem from several perspectives, including discussions of photocatalysis, multifunctional nanoparticle catalysts, materials for water splitting, and novel fuel cell materials.

The day began with opening comments by Symposium Chair and Materials Science Program Director Todd Krauss. The first talk of the morning, “Rational Synthesis of Metallic Nanoparticles for Catalytic Applications,” was given by Dr. Shouheng Sun. Professor Sun joined the Chemistry Department of Brown University in 2005, and currently serves as the Co-Director of Brown’s Institute for Molecular and Nanoscale Innovation (IMNI) and as an associate editor to the journal “Nanoscale” (the Royal Society of Chemistry). The second seminar of the day, “Catalysis synthesis: Beyond art, but a highly underexplored [and non-linear] science” was presented by Dr. Robert M. Rioux. Robert Rioux is currently the Friedrich G. Helfferich Assistant Professor of Chemical Engineering at the Pennsylvania State University. The morning program ended with the talk “Stable and functional hybrid interfaces via bilayered molecular systems” by Dr. Alexander Shestopalov, an Assistant Professor in the Department of Chemical Engineering at the University of Rochester. Alex started his academic career at the University of Rochester in early 2010, and his research interests include studying the properties of hard and soft



From left (back): James Muckerman, Oleg Prezhdo, Robert Rioux, From left (front): Todd Krauss, Shouheng Sun, Peng Chen

material interfaces and how they can be modified and structured using organic and polymeric materials.

The afternoon program kicked off with Dr. James Muckerman, Deputy Chair for Strategic Planning, and Senior Chemist in the Chemistry Department of Brookhaven National laboratory in Upton, New York. He spoke about a very popular topic: “Photocatalytic water oxidation at the GaN (10 $\bar{1}$ 0) – water interface.” By creating a new catalyst capable of converting hydrogen gas and carbon dioxide to liquid formate at room temperature, this storage system could revolutionize the ways in which hydrogen is transferred and stored. As a continuation of this topic, the next speaker, Alexey V. Akimov, presented his research on “Non-adiabatic dynamics of photoholes during initial steps of the photocatalytic water splitting on GaN(10-10) surface: Charge localization governs splitting efficiency.” Alexey has been working with Prof. Oleg Prezhdo’s group at the University of Rochester, and in 2012 he joined a collaborative project with Dr. James Muckerman at the Department of Chemistry at Brookhaven National Laboratory. The final speaker of the day was Dr. Peng Chen, a Professor in the Department of Chemistry and Chemical Biology at Cornell University. The topic of his presentation was “Single-nanoparticle catalysis at single-turnover and nanometer resolution.” Professor Chen began his faculty appointment at Cornell University in 2005 and his research focuses on single-molecule imaging of nanoscale catalysis, as well as of metal homeostatic machineries both in vitro and in vivo.

The 2013 Chemistry-Biology-Biophysics Cluster Retreat

One goal of the Chemistry-Biology-Biophysics Interface Training Cluster is to increase interactions between groups doing Chemistry, Biology, Biochemistry, and Biophysics at the University of Rochester. The Cluster currently has research groups from the Departments of Chemistry (13), Biology (3), Biochemistry & Biophysics (10), Microbiology (5), and Pharmacology (1). The main medium for achieving the Cluster's goals is an annual Retreat that is largely funded by the University Committee for Interdisciplinary Studies (UCIS).

This year, the Retreat started on the afternoon of June 6 with a talk by Prof. Eric Kool (George and Hilda Daubert Professor of Chemistry, Stanford University) to an audience of about 100 people in Lander Auditorium in Hutchison Hall. The talk was titled: "Designer DNA Bases as Probes for Biological Molecules and Processes." Dr. Kool first described the organic chemistry and combinatorial screening approach for discovering DNA tetramers with combinations of unnatural "bases" that produce novel fluorescence and binding properties. He then described applications to imaging in cells and to detection of ions. Thus, his talk encompassed the Retreat's theme of interdisciplinary research combining chemistry, biology, and biophysics.

Prof. Kool started his independent research in 1990 as a faculty member in UR's Department of Chemistry and moved to Stanford in 1999. This was his first return to Rochester and, therefore, the first opportunity for biological groups to hear about applications of his new materials.

The Retreat reconvened at the Staybridge Suites Hotel at 9:30 AM the next day with 84 attendees. The day started with fruit, juice, coffee and breakfast pastries and a session of 15 posters

ranging from synthesis to computations, with a wide variety of studies in between. This was followed by a buffet lunch, six scientific talks, and a very informative "Career Panel Discussion," that included Eric Kool, Payel Das (IBM), Sina Ghaemmaghami (Assistant Professor, UR Biology), Josh Blose (Assistant Professor, SUNY Brockport), Brian Edelbach (Assistant Professor, Monroe Community College), and Hal Ebetino (retired from Proctor and Gamble and currently involved with biotechnology start-ups). Drs. Edelbach and Ebetino received their Ph.D.s from UR's Department of Chemistry and Dr. Blose did his Ph.D. research with Prof. Phil Bevilacqua at Penn State. Phil did his Ph.D. research at UR. The participants provided interesting histories of how they made career choices. Valuable advice was given on what employers look for when hiring. Many questions from students pertained to academic positions. Three graduate students gave talks on their research. The students represented the Department of Chemistry, the Department of Biochemistry & Biophysics, and the Department of Pharmacology and Physiology. Fifteen students and postdocs presented posters on their research in a lively poster session in which poster presenters interacted with students and faculty from many different departments and groups as well as with the visiting scientists.

Much information was exchanged throughout the two days and new connections were made that can enhance research and training at the Chemistry-Biology-Biophysics Interface at UR. Several attendees were undergraduates participating in summer Research Experience for Undergraduates programs.

The Retreat gave all participants a broad overview of research related to biology and an appreciation of interdisciplinary approaches.



Doug Turner, Hal Ebetino, Kara Bren, Eric Kool, Brian Edelbach, Sina Ghaemmaghami, Payel Das, Alan Grossfield

Two Teaching Awards - Frontier & Hafensteiner

Professor Alison Frontier received the 2012 Goergen Award for Excellence in Undergraduate Teaching

in recognition for her excellence in teaching the large organic chemistry course, CHM 204, in addition to the other classes she has taught since joining the faculty at UR. 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.



Alison joined our faculty in January 2002 after completing her Ph.D. in 1999 (Organic Chemistry, Columbia University) and postdoctoral work at Stanford University (1999-2001). Professor Frontier has been exceptionally productive during her time here, publishing numerous articles in premier journals, attaining significant results in a science that is often characterized as incremental in nature, and has, additionally, acquired significant, external funding from both the NIH and the NSF. Robert Boeckman, chemistry department chair, says “Alison is rapidly being recognized as one of the outstanding chemists in her cohort in the field of synthetic methods development and complex molecule synthesis. She is an engaging and exciting lecturer, a thorough and dedicated mentor, an accessible and knowledgeable instructor.”

Established in 1997 by University Trustee Robert Goergen and his wife, Pamela, the Goergen Award for Excellence in Undergraduate Teaching (formerly the Goergen Award for Distinguished Achievement and Artistry in Undergraduate Teaching) recognizes the distinctive accomplishments and skills of individual teachers in undergraduate courses in the College. The Award aims to recognize the full scope of educators’ work that contributes to excellence in undergraduate education. The award was presented to Professor Frontier at a special luncheon and award ceremony held in the Multi Activity Center (Goergen Athletic Center) during Meliora weekend, Friday, October 12, 2012.

Dr. Ben Hafensteiner was named Professor of the Year in the Natural Sciences,

an award bestowed on behalf of the University of Rochester Students’ Association who determined, after a careful screening of the pool of nominations, that Ben best fulfilled the criteria for this high honor.

The Students’ Association Professor of the Year Award was created in 1981 to increase awareness of the importance of undergraduate instruction. The program recognizes faculty members for their achievement purely as an undergraduate professor. The award is given annually to recognize a faculty member in each academic division of the College (Engineering, Humanities, Natural Sciences, and Social Sciences) who makes a positive and lasting impact on undergraduate student life at the University through dedication to developing relationships with students, creation of an engaging and challenging classroom atmosphere, as well as inspiring the further pursuit of knowledge.



Ben received his B.A. degree in Chemistry here at the UR in 2003 and his Ph.D. from The Scripps Research Institute in 2008. He and his wife moved to the Rochester area two years ago when Ben began lecturing in general and organic chemistry each semester.

Students raved about Ben’s ability to make any class feel small even though they were generally large lectures. They also explained how supported they feel by Ben as a mentor outside of the classroom. It’s clear Ben’s students have a profound respect and appreciation for his knowledge and enthusiasm. To honor Ben, he was invited to attend the Undergraduate Research Expo on Friday, April 19, 2013 where he was presented with this award.



ACS on Campus at Carlson Library

The American Chemical Society (ACS) has an outreach program called **ACS on Campus** “dedicated to helping students, post-docs, and faculty members advance in their careers”. A planning committee of Sue Cardinal, Chemistry Librarian, James Shanahan, president of the Undergraduate Chemistry Council (UCC), Michael Baranello, graduate student in chemical and biomedical engineering, Dr. Will Eckenhoff, postdoc and member of the Younger Chemist Committee (YCC), Prof. Udo Schroeder, faculty, Robin Cooley, administrative assistant, and Jennifer Taylor Howell, from ACS worked together to plan this event.

On Monday, April 15, at MacGregors in Henrietta, we held a Science Café networking reception for students, faculty and the local science community. The next day, April 16, sixty-five chemists, librarians and entrepreneurs from University of Rochester and beyond came to Carlson Science & Engineering Library for a full day program. One librarian joined us from Lithuania! Sue Cardinal, Chemistry Librarian and Dr. Robert K. Boeckman, Jr., the chair of the UR Chemistry Department and Associate Editor for the *Journal of Organic Chemistry*, welcomed everyone to Rochester.

Next, Prof. William D. Jones, UR faculty and Associate Editor of the *Journal of the American Chemical Society*, covered the “Basics in Scholarly Publishing”. This was a



Bill Jones, UR Chemistry

heart to heart talk to students about how to thoughtfully prepare their papers from the context of what will happen once your paper is submitted. This was followed by Dr. Sonja Krane, Managing Editor of *Journal of the American Chemical Society*, who spoke about “Copyright and Ethics in Scholarly Communication: What You Need to Know”

and John Kratunis (M.S. '83) from CAS, who discussed the current version of SciFinder in “The SciFinder® Advantage for Your Career”.

After a brief boxed lunch, Dr. Sonja Krane returned to introduce us to the recently released ACS ChemWorx, a fully featured reference manager in “ChemWorx Presentation: From Inception to Collaboration to Publication.” There are plans to add project management software and links to ACS Paragon Plus, the publishing platform for ACS. An iPhone app can now be downloaded.

Dr. Duncan Moore, Vice Provost of Entrepreneurship from the UR, Michael Riedlinger, Rochester BioVenture Center Program Manager from High Tech Rochester, Mark Palvino (B.S. Optics) from Optimax and Rami Katz, Chief Operating Officer of Excell Partners, Inc. participated in an engaging panel discussion about the numerous opportunities available to the University of Rochester community. The program was called “Entrepreneurship in Upstate New York: What You Need to Know to Start Your Own Venture.” Right before the closing reception, Dr. Patrick Gordan from ACS presented a hands-on program called “ACS Career Pathways: Finding Your Path In Industry and Government.”

Special Note:

We invite you to come visit Carlson Library

to see the second floor renovation! This past summer, in order to create space for collaboration with technology, the circulation desk was cut in half and refinished to feature an oval shaped table with two large back to back displays. One to four people can connect their laptops to each

display. Colorful and playful seating was added in front of the desk. Clean windows, new paint on the walls and in the stairwell and fresh carpet complete the new look.



Student Awards and Accolades

Pictured with Professor Brad Nilsson (left below) is the John McCreary Memorial Prize winner, **NATHANIEL BROWN, JR. (B.S. '13)**. This prize was established in 1985 in tribute to the high academic and scientific standards, and the personal dedication of John James McCreary who received his B.S. degree in Chemistry in 1975. Nate, who graduated with the chemistry department's highest distinction honors and was elected to Phi Beta Kappa, has now started graduate studies in chemistry at Princeton University.



This year there were two recipients of a Carl A. Whiteman, Jr. Teaching Award - **NATHANIEL BROWN, JR. (B.S. '13)** - pictured above - and **BENJAMIN HYERS (B.A. '13)**. This award recognizes exemplary teaching by an undergraduate student in the department of chemistry. Ben, Phi Beta Kappa and highest distinction honors in chemistry, worked with Professor Alison Frontier and is attending medical school.

MICAH BROWN (B.S. '13) also graduated with chemistry department highest distinction honors and is a member of Phi Beta Kappa. Micah was the recipient of the Dr. E.W. and Maude V. Flagg Award. This award was established in 1982 as an endowed fund by Dr. John J. Flagg to recognize outstanding performance and promise in chemistry by a graduating senior. Micah completed undergraduate research with Professor David McCamant, studying computational methods and Raman spectroscopy. He is now attending the University of North Carolina at Chapel Hill to pursue a doctorate in analytical chemistry.

JOSEPH COLARUOTOLO (B.S. '13), received the 2013 ACS Rochester Section Award given to a senior with an outstanding academic record. He was recognized during the ACS Annual Rochester Section Undergraduate Research Symposium and his name is now displayed on a plaque in the department.

Joe enjoyed working with Professor David McCamant on the excitation dynamics of P3HT and graduated with chemistry highest distinction honors. He is attending the University of Chicago to pursue a Ph.D. in chemistry.

Each year the American Chemical Society (ACS) gives an Inorganic Chemistry Award to a student who is selected by the faculty on the basis of outstanding academic achievement in inorganic chemistry. **LUXISHEN (B.A. '13)**, this year's award winner, worked tirelessly in Professor Richard Eisenberg's lab on the development of catalysts for proton reduction. Luxi is pursuing a Ph.D. at Cornell University. New this year from the ACS, is an Organic Chemistry Award, won by senior **JARED NESVET (B.A. '13)** - highest distinction and Phi Beta Kappa. Jared worked with Professor Mike Neidig synthesizing and spectroscopically analyzing various iron-based catalysts and is continuing to pursue these spectroscopic interest in biological systems with Professor Ed Solomon at Stanford University.

Chemistry Department awards went to **JOSHUA BIELEMEIER, (B.A. '13)**, **ALISON HAMLIN, (B.S. '13)**, **BENJAMIN HYERS (B.A. '13)**, **NICHOLAS JACOB (B.S. '13)**, **RACHEL KELEMEN (B.S. '13)** and **ZACHARY PRESSMAN (B.A. '13)**. These awards are given to seniors in recognition of outstanding scholarship in the study of chemistry.

ALISON HAMLIN (B.S. '13) also received the Janet Howell Clark Prize. Established by the University, this award is given to the senior woman who has shown the greatest promise in creative work in one of the following fields - Physics, Chemistry, Biology, or Astronomy - and has shown outstanding versatility in the mastery of allied fields. Alison graduates with the highest distinction chemistry honors and was elected to Phi Beta Kappa. She had previously been awarded the Merck Index Award for Outstanding Achievement in Organic Chemistry. Alison spent three semesters conducting research on solar hydrogen production in Professor Rich Eisenberg's lab, as well as studying abroad one semester in Kenya where, for one month in the field, she studied the social and economic impact of biogas digester use.



Rising senior **HEE YOUNG (RACHEL)** received the Catherine Block Memorial Fund Prize. This University award is given to a woman in the Junior class in recognition of her outstanding ability and achievement in the field of science. The student award winner is recognized during the first fall chemistry department get together.

The Edward Peck Curtis Award for Excellence in Teaching by a Graduate Student is a University wide competition given to exceptional teaching assistants. **KIMBERLY MANBECK**, now in her fourth year in Professor Jone's lab, was among the graduate students across the University who received the 2012 award. The nomination includes letters of support from the chair, faculty and students. The comment heard from students many times about Kim is that "she is an excellent teacher, kind, considerate, and fully invested in her students. She is helpful, approachable, and wants her students to succeed."

YICK CHONG LAM (B.S. '13) was chosen to receive the CRC Press Chemistry Achievement Award for a Senior based on outstanding accomplishment in chemistry. Yick graduates with the department's highest distinction of honors. Yick conducted research with Professor Fasan on designing alternative strategies for synthesizing Macrocyclic Organo-Peptide Hybrids (MOrPHs). Yick began his graduate studies in chemistry this fall at Yale University.



As noted in an interview for the *Career & Internship Digest* of the UR Gwen M. Greene Center Yick mentions that "during freshman honors organic chemistry, I became interested in designing molecules with therapeutic properties . . . "My one piece of advice: Always pursue your interests and keep learning in any and every environment. Do not hesitate to ask professors for research opportunities or even to ask questions during class," he says.

The department gave five W.D. Walters Teaching Awards this year: **ADAM FEINBERG (M.S. '13)**, **JEFFREY KEHL**, **JARED KNEEBONE (M.S. '13)**, **GILBERT REYNDERS (M.S. '13)**, and **JAMES VIRNELLI, III (M.S. '13)**. This award, memorializing the late Professor Walters, recognizes outstanding undergraduate teaching by graduate teaching assistants and their commitment and achievements.

BREANNA ENG (B.A. '13) received a special chemistry department award to honor her outstanding effort and contributions on behalf of the department. Breanna has been a student office assistant specifically for the Undergraduate Studies and Development Administrators where she has used her design and computer skills to create most of the posters, brochures, covers and other artwork seen and used throughout the department - including the cover of this newsletter! Throughout her four years here, Breanna was very involved in student activities, Track & Field, Campus Crusades, VP of Marketing for the Riverview Hall Council, and took a semester to study abroad in New Zealand as a Gilman scholar. Breanna is attending the Warner School here at the UR to earn her Master's degree in secondary education in chemistry with a certification to teach children with disabilities in an inclusive classroom.



RUJA SHRESTHA (PH.D. '12), was selected to receive a commendation in the Outstanding Dissertation Award competition for the natural sciences, a testament to her exceptional work as a graduate student at the UR with Professor Dan Weix. Ruja is now at the University of California, Berkeley, in the John Hartwig group to further her skills in organometallic chemistry and is currently investigating transition-metal-catalyzed oxidative olefination of arenes.



Congratulations to rising seniors **SARAH KONISKI** (Bren group) and **LOUIS PAPA** (Fasan group) who spent their summer conducting research in German laboratories through the German Academic Exchange Service-Research Internships in Science & Engineering Scholarship (DAAD-RISE) program. Louis plans to graduate from Rochester and pursue a doctoral degree in chemical biology and medicinal chemistry and hopes to teach at the university level. He interned at the Institute of Organic Chemistry and Macromolecular Chemistry at the University of Jena, while Sarah spent her time at the Jülich Research Center (Forschungszentrum Jülich) adding to

her general knowledge of computation chemistry while testing different computation methods for radionuclide-bearing molecules. While her post-graduation plans are still undecided, she is interested in enrolling in a master's degree program in chemistry or pursuing an industry career.

DAVID GEORGE (B.S. '13) won the President's Award for Undergraduate Research in the Natural Sciences at the spring Undergraduate Research Symposium. David worked in Professor Dan Weix's lab under the direction of graduate student Dan Everson, investigating the synthesis of a naturally occurring molecule found in the fungus *Cephalosporium recifei*. George is attending the University of California, Irvine to pursue a Ph.D. in organic chemistry.

In the college writing contest, **YICK CHONG LAM (B.S. '13)** (Fasan group, pictured on pg 21), received an Honorable Mention in the Natural & Applied Sciences Division for his paper entitled "Evolution of Nuclear Drug Delivery" written for CHM 440 (Nilsson).

David George with President Joel Seligman at award ceremony



See also **Commencement** beginning on page 60

Masters Degree recipients at the 2013 Commencement Ceremony (not all are pictured here)

Stephanie Daifuku, Gilbert Reynders, Adam Feinberg, Megan Reesbeck, Malik Al-Afyouni, Nicholas Arnet, and Jared Kneebone



Robert K. Boeckman, Jr.

Marshall D. Gates, Jr. Professor of Chemistry and Chair

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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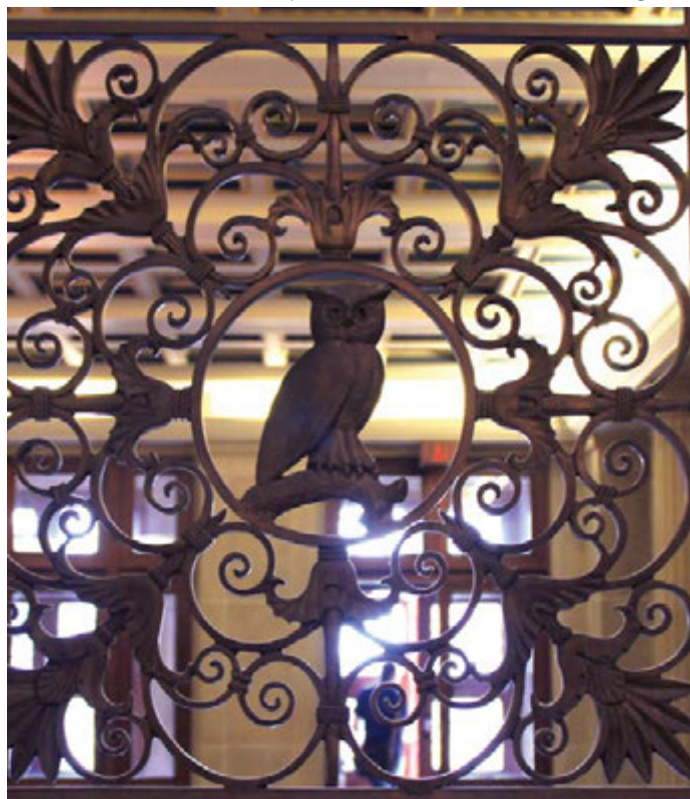
During the 2012-2013 academic year, **ROBERT K. BOECKMAN, JR.** completed his tenth and final year as the chair of the chemistry department. He continues his duties as associate editor of the *Journal of Organic Chemistry*, and is now President and Chair of the Board of Directors of Organic Syntheses, Inc.

Bob Boeckman's research group continues 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 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 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 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 α oxidation of aldehydes and other applications. New collaborative projects have been initiated with Professors David Goldfarb of the biology department and Damian Krysan of the Department of Pediatrics, URM, 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 PDK-1 inhibitors showing specificity for the fungal enzymes for use in antifungal therapy against invasive fungal infections of neonatals and young infants.

GREG FRATTINI (PH.D. '10) continues as a postdoctoral associate in the group working on the Goldfarb (biology) collaboration. **NATHAN E. GENUNG (PH.D. '10)** joined Pfizer Inc. in Groton, CT as a research scientist. **XINYI SONG (PH.D. '07)** continues to be employed as a research chemist with J&W Pharmed in Levittown, PA. **GEORGE ARAB (PH.D. '13)** defended his thesis in June and will

Metal Sculpture in Rush Rhees (Breanna Eng '13)



join the group of Dean Toste at UC Berkeley as a Post Doctoral Associate in November 2013. **MATT BETUSH (PH.D. '13)** defended his thesis in September 2013 and as of August joined the faculty of Allegheny College as a Temporary Visiting Assistant Professor. Part-time scientist Dr. Dennis Savage, retired from Kodak, continues his work in the group on several projects with the Goldfarb (biology) and Krysan groups (pediatrics URMC). Sarah Paulson and Hui Wang are completing their 4th year. Sarah is working on CBS catalyzed enantioselective Mukiyama aldol reactions, and Hui on the total synthesis of Nakadomarin assisted by entering first year student Kyle Rugg (RIT BS/MS). Douglas Tusch and Kyle Biegasiwicz, now completing their 3rd year, have just completed their doctoral requirements and are focused on research. Doug has taken over apoptolidin from Brian Ohman, and Kyle has taken on FK-506 assisted by beginning 2nd year student Lifeng Xiao. **COLE CRUZ (B.S. '13)** and **JESSICA WEBER (B.S. '13)** completed their B.S. theses in the group in Spring 2013. Cole began graduate studies in chemistry

at UNC Chapel Hill this fall and Jessica will pursue a high school chemistry teaching career. Gilbert Reynders (Lake Forest College) joined the group in December 2011 and is working on extensions of Matt Betush's work on catalysis including asymmetric versions using Chromium(II) and Copper(I). **CHRISTINA COLLISON (PH.D. '04)** continues as associate professor of chemistry at RIT and **JEREMY CODY (PH.D. '04)**, was promoted to associate professor of chemistry also at RIT. **JOSEPH PERO (PH.D. '05)** continues as a research scientist with Merck in West Point, PA. **XIAORONG LIU (PH.D. '04)** continues as a research scientist at Astra-Zeneca in Waltham, MA. **JING ZHANG (PH.D. '02)** and **JONATHAN LAWRENCE (B.S. '02, PH.D. HARVARD '08)** continue as Senior Research Scientists at Cubist Pharmaceuticals in Lexington, MA. **TODD R. RYDER (PH.D. '05)** after a year as a visiting Assistant Professor at Wesleyan University, joins Quinnipiac University in Connecticut for a one year appointment as an Assistant Professor of Chemistry with a tenure track position likely after that year.

Hoyt Auditorium (Moxi Zhou '13)



Kara L. Bren

Professor of Chemistry

Ph.D. 1996, California Institute of Technology



RESEARCH INTERESTS

Bioinorganic and biophysical chemistry: heme protein structure and function, protein folding and dynamics, NMR of paramagnetic biomolecules, solar energy conversion.

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The **KARA BREN** group is continuing their studies on cytochrome c biochemistry and on engineering cytochromes for applications in energy conversion. Jesse Kleingardner, the senior student in the lab, is wrapping up his thesis work with his exciting result on a cytochrome c-derived catalyst for efficient electrocatalytic reduction of protons to water. After defending his thesis, Jesse will be moving to Ithaca where he will be a Postdoctoral Teaching Fellow at Ithaca College. Jesse will have the opportunity to continue his research in the area of protein-derived catalysts while at Ithaca. Lenore Kubie, a joint student with the Krauss lab, is continuing her work on photoinduced electron transfer from cytochrome c derivatives to nanotubes. This summer, she traveled to Ghana with the NSF IGERT Program. In May, graduate student Becky Smith presented her results on the effects of electronic structure on electron transfer reactions in cytochromes at the Canadian Biological Inorganic Chemistry (CANBIC) conference in Parry Sound, Ontario. In upcoming work she will be applying biological electron transfer reactions for applications in energy conversion. Graduate student Banu Kandemir is investigating proton-reduction catalysts and has discovered a metallo-peptide-based catalyst that she will be developing further. Banu also is collaborating with Zhiji Han in the Eisenberg group developing photocatalytic systems for hydrogen evolution from water using biomolecule-derived catalysts.

The Bren group saw two senior thesis students graduate this year. **BENJAMIN DICK (B.S. '13)** has been developing heme peptide derivatives with altered reduction potentials and will be continuing this work as a 5th-year Master's student as he develops his compounds for catalysis. **HOON KIM (B.S. '13)** studied the effects of cytochrome c structure on heme electronic structure and has returned to his native Korea.

We received some exciting news from Bren group alumni. Former postdocs **MATTHEW LIPTAK (POSTDOC '12)**

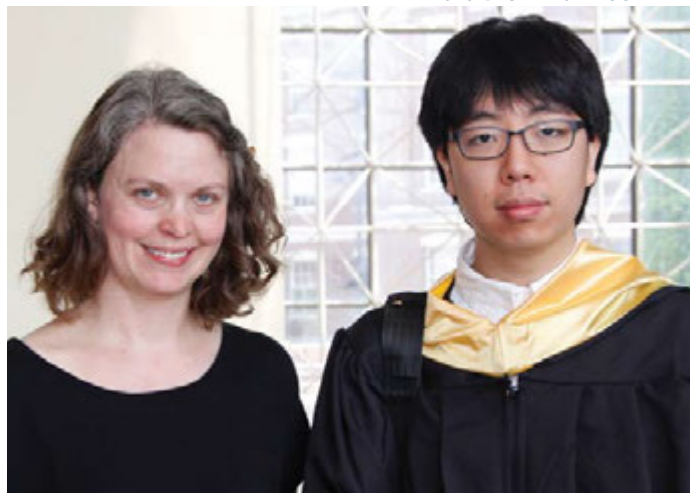
Kara Bren presenting Benjamin Dick his diploma



and **ANDREA LEE (POSTDOC '12)** welcomed a baby girl, Jacqueline. Matt and Andrea are currently at the University of Vermont. Another former postdoc, **ANNI SIITONEN (POSTDOC '12)**, accepted a job as Senior Scientist at Polestar Technologies in Boston.

Kara has enjoyed her travels over the past year, which included attending the Metals in Biology GRC in Ventura, CA, a workshop on spin states of transition metals in Zaragoza, Spain, and the Korean Chemical Society meeting in Seoul, Korea.

Kara Bren with Hoon Kim



Esther M. Conwell

Research Professor

Ph.D. 1948, University of Chicago



RESEARCH INTERESTS

Transport along the base stack in DNA; proton transfer in DNA; electrical and optical properties of organic semiconductors, particularly conjugated polymers.

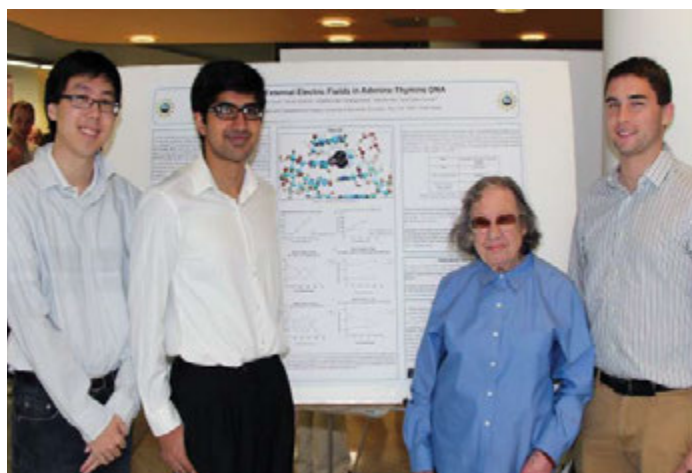
CONTACT

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ESTHER CONWELL: A recent publication claims to show that a high electric field acting on a guanine, G, paired with a cytosine, C, can cause the transfer of a proton from G to C. [Kinz-Thompson-Ceron-Carrasco and Jacquemin, *PhysChem-ChemPhys*, 2013, 15, 4548, to be abbreviated C-C and J] In particular, in their simulations they find that the proton shifts from its canonical position close to nitrogen N1 of guanine to the position close to N3 of cytosine for a field 80 to 100×10^{-4} au, or 4 to 5×10^9 volts/m. The field must be directed parallel to the hydrogen bonds pairing G and C. Attempting to check their results, we set up a chain of G/Cs, applied a high electric field, and set up a simulation for this situation using the computer code CP2K. We found, unexpectedly, that application of the field caused the temperature of the DNA and the water to rise rapidly after a few femtoseconds. We guessed that the rapid rise was due to the action of the high electric field on the water. This was verified by the fact that similar heating occurred in a run with the water in the field without the DNA. We believe that the difference between our simulated results and those of C-C and J are due to the fact that they approximated the water with a continuum model, whereas the code we used treats the water as H_2O molecules. Of course, it is still necessary to make approximations in treating the water molecules. For the simulations we used, which involved 3000 water molecules, the waters were treated in the popular TIP3P model. It is noteworthy that a straightforward calculation of the temperature rise for a field

of 100×10^{-4} au, using experimental values for the resistivity and the specific heat of water, gave a result less than 1 degree for 25fs water exposure. This suggests that the TIP3P water model does not give a good representation of the properties of water that determine its resistivity and/or specific heat. We will investigate this situation further.

In earlier simulations we had found that proton transfer occurs in an adenine, A, paired with a thymine, T, over a wide range of temperatures below room temperature, but not at room temperature ($\sim 300K$). [Kinz-Thompson and Conwell, *J. Phys. Chem. Lett.* 2010, 1, 1403] The proton moves from being close to N6 of adenine to being close to O4 of thymine. We decided therefore to investigate whether a high electric field could cause proton transfer in A/T from adenine to thymine at 300K. We found that in a field of 20×10^{-4} au, $\frac{1}{4}$ of that where proton transfer due to the field was reported by C-C and J, the temperature of the water also rose. The rise could be avoided by introducing into our calculations a thermostat to keep the water temperature close to 300K. The thermostat we used, CSVN (Canonical Sampling through Velocity Rescaling), which is included in CP2K, reduces the temperature by reducing all velocities by the same factor. With the thermostat applied periodically at short intervals the temperature was kept reasonably constant, and the proton was found to move in short steps over almost half the distance between A and T. In a field half as large, 10×10^{-4} , we found the proton did not move at all. These observations give a measure of the height of the barrier for the proton between A and T in the A/T molecule. This work is being continued.



This summer Esther had several REU students (from chemistry and physics), shown here with three. Among other awards and honors received throughout her long career, Esther is the recipient of a Camille and Henry Dreyfus Senior Mentor Award (2005), the Susan B. Anthony Lifetime Achievement Award (2006), and the 2008 ACS Award for Encouraging Women into Careers in the Chemical Sciences, as well as a National Medal of Science (2010).

Joseph P. Dinnocenzo

Professor of Chemistry

Ph.D. 1983, Cornell University



RESEARCH INTERESTS

Chemistry of organic ion radicals; mechanistic and physical organic chemistry; electron transfer reactions

CONTACT

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JOE DINNOCENZO and his group continue to pursue a variety of problems in electron transfer and related chemistry. In collaboration with Samir Farid, former postdoc **DEEPAK SHUKLA (POSTDOC '00** - Eastman Kodak), and Dr. Shashi Adiga (also at Kodak), we recently investigated the chain amplified photochemical fragmentation of N alkoxy pyridinium cations in the presence of pyridine bases. As part of this chemistry, we discovered a novel reaction between alkoxy radicals and pyridine bases in which a hydrogen atom is transferred from the alkoxy radical to the pyridine base. Quantum chemical calculations indicated a proton coupled electron transfer mechanism for this unusual hydrogen atom transfer. We are currently investigating the generality of this new reaction.

Graduate student Adam Feinberg is working on understanding the general mechanism for fragmentation of aryltrialkyl Group 14 cation radicals. Adam has discovered that similar to aryltrimethylstannane cation radicals (previously investigated in the group by **PU LUO, PH.D. '12**), aryltrimethyl silane and germane cation radicals undergo fragmentation to preferentially give the less stable aryl radical rather than a methyl radical. Adam is currently working to fully understand the mechanism of these reactions. Adam also completely rewrote our computer programs to control new excimer and dye lasers that we installed on the group's nanosecond transient absorption apparatus over the past year.

Joe is continuing work with graduate student Terrell Samoriski on a pedagogical research project involving the design, implementation, and evaluation of the Peer Led Team Learning (aka Workshops) model for CHM210 (Honors Organic Laboratory II). Among other things, Terrell's research has shown that students find Workshops help them better prepare for lab and improve their data analysis – two perennial problems experienced in laboratory courses.

Joe also had the pleasure of working with Profs. Philippe Hiberty (Université de Paris- Sud) and Benoit Braïda (Université Paris '06) to complete a project on the nature of multicenter bonding in the ditetracyanoethylene dianion. Joe previously spent part of a sabbatical with Philippe to learn how to do valence bond calculations.

Clock Tower in Dandelion Square



Richard Eisenberg

Professor of Chemistry / Research Professor

Ph.D. 1967, Columbia University



RESEARCH INTERESTS

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

CONTACT

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It has been another banner year for **RICH EISENBERG** and his research group. "Researchwise," notable progress was made in developing and analyzing new systems for the photogeneration of H₂ from water. This reaction is the reductive side of splitting water into its constituent elements and is the key reaction for light-to-chemical energy conversion in artificial photosynthesis. During the past year, a new system based on collaborative work with Pat Holland and Todd Krauss on the use of CdSe quantum dots as the light absorber was reported in *Science*. The catalyst in this system was a simple Ni complex in solution. The individuals really responsible for this work were grad students Zhiji Han and Fen Qiu of the Krauss group. This highly regarded work has set the Eisenberg group in a new direction on the modification of quantum dot surfaces to make such systems more durable and amenable to examination with other catalysts. This work is being carried forward by new postdoc Amit Das

Rich's final meeting with the Editors of Inorganic Chemistry in December (left to right): Rich, Jim Mayer, Vivian Yam, Vince Pecoraro, Ed Solomon, Frank Meyer, Kim Dunbar, Alan Balch, Bill Tolman



and visiting graduate student Mohsen Haghghi (from Iran), as well as Zhiji. Other work on different Ni catalysts was completed and studies on dithiolene complexes of Co and Mo are continuing. Graduate student Randy Sabatini, who is co-advised with Dave McCamant, has also made significant progress in looking at ultra-fast processes involving dye sensitizers attached to TiO₂ for H₂ generation. This research is supported by NSF in a collaborative project with University at

Buffalo scientists. Lastly, graduate student Ryan Cheng, who is jointly advised with Alison Frontier, has followed up initial observations by **TULAZA VAIDYA (PH.D. '12)** last year on a new recyclable heterogeneous gold catalyst for electrocycloization reactions.

Travels are always part of the annual happenings for Rich. In September, he and Marcia traveled to London for several days of vacation just after the Olympics and then Rich traveled on to Sheffield to speak and participate in the Dalton Discussion Meeting on Inorganic Photophysics and Photochemistry – Fundamentals and Applications. Following his return, he (and Marcia) headed out to Vancouver to experience the beauty of British Columbia and give lectures at the University of Victoria, University of British Columbia and Simon Fraser University. The real highlights of the year, however, were the very special occasions associated with receiving the Fred Basolo Medal at Northwestern University in October and the William H. Nichols Medal from the New York Section of the American Chemical Society in March. The Basolo medal was particularly meaningful because Rich is a "scientific grandson" of Fred's and knew Fred for many years. The awarding of the Nichols Medal was coupled with a symposium in which Harry Gray, Cliff Kubiak, Bill Jones and Marcetta Darensbourg all participated. It was a great event and allowed Rich to share the moment with these close friends and with all of his family (in black tie, no less).

In December, 2012, Rich finished his term as Editor-in-Chief of *Inorganic Chemistry*. After a dozen years, Rich thought it was time to turn over the reins. During his tenure, the journal made great gains in total citations and impact factor, and solidified its position as the #1 journal in its field for the reporting of new research. At the annual ACS Editors Conference in January, 2013, he was recognized by his fellow editors and had an opportunity to thank all who helped make his editorship successful. Key among these folks was Arlene Bristol who has worked with Rich for more than 20 years and who was the chief editorial assistant during his term with IC. Arlene began working for ACS Publications more than 50 years ago with Albert Noyes and Marshall Gates when the *Journal of*

the American Chemical Society was edited at Rochester. After spending time at the University of Michigan and Princeton University, Arlene returned to Rochester in 1990 and began working with Rich, Jack Kampmeier and other faculty before becoming the chief journal assistant and Coordinating Editor for IC. In November, 2012, just ten weeks before retirement, Arlene came down with a form of leukemia. Fortunately, with great doctoring and her characteristic determination and grit, the disease is now in remission, and after a 6-month leave, Arlene was able to return to work to close down the Inorganic Chemistry EIC office in May with Rich. A happy ending to a very successful run. As for Rich, he is not out of the editing business entirely. In May, he became an Associate Editor for the *Proceedings of the National Academy of Sciences*.

Group comings and goings during the past year include the arrivals of postdoctoral Amit Das, student Mohsen Haghghi

and Atsushi Kobayashi, a visitor from Japan who spent 3-months in the Eisenberg laboratory. The departures of the past year all came through graduation in May of a wonderful group of undergraduates who worked in the Eisenberg laboratory over the past year. They include **LUXI SHEN (B.A. '13)** who is going to Cornell for graduate school, **TROY (LIDONG) WANG (B.S. '13)** who is going to continue for another year to get his M.S. degree here, **ALISON HAMLIN (B.S. '13)** and **MIKAEL OLEZESKI (B.S. '13)** who will do a 'Take-Five year in Italy (great work if you can get it). Rich was delighted to have these undergraduates in the group, as they kept a steady stream of questions and enthusiasm flowing in the laboratory. Despite the absence of departures at the postdoc level, substantial change will occur in the coming months with Will Eckenhoff taking a faculty position at Hobart and William Smith Colleges and the arrival of two new postdocs.



Celebrating the graduation of four undergraduates, May 2013

Samir Farid

Research Professor

Ph.D. 1967, Göttingen University



RESEARCH INTERESTS

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

CONTACT

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The focus of **SAMIR FARID**'s research continues to be on electron transfer reactions and kinetics. During the past year mechanistic and theoretical studies of highly chain-amplified photochemical reactions of N-alkoxy-pyridinium salts were carried out in collaboration with Deepak Shukla (Eastman Kodak) and Joe Dinnocenzo. The work was published in

a JOC article in which it was proposed that alkoxy radicals react with pyridine bases via proton-coupled electron transfer to form pyridinyl radicals (a net hydrogen atom transfer). This process may have implications in biological systems, where traditionally hydrogen atom transfer to, not from, alkoxy radicals is the accepted mechanism.

James M. Farrar

Professor of Chemistry

Ph.D. 1974, University of Chicago



RESEARCH INTERESTS

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

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“Radicals in the lab” has been the theme for JIM FARRAR and his research group during the past year. The group’s first paper on ion imaging, published in the *Journal of Chemical Physics*, was selected as an Editors’ Choice publication for 2012. Our initial work has focused on the ion-molecule chemistry of carbon- and nitrogen-based cations with methane and ammonia. Jim had an opportunity to present some of this work at the ACS meeting in New Orleans, and will participate in the inaugural symposium of the newly-formed Astrochemistry subdivision of the Physical Chemistry division at the Indianapolis ACS meeting this September. His talk, on the ion chemistry that initiates ion processing in the atmosphere of Titan, Saturn’s largest moon, cements his reputation for being ‘lost in space.’

Thanks to postdoc Linsen Pei, we now have a working ion-radical experiment, and some of our initial work with methyl radicals has been ‘odd’ indeed! It is clear that the relatively unexplored area of ion-radical chemistry holds many surprises, and with the continuation of support from the National Science Foundation, we look forward to delving into these mysteries. This summer, we have been joined in the lab by REU student Brian Barker from UR as well as Dr. Stefano Falcinelli from the University of Perugia in Italy. Stefano’s visit maintains a tradition of collaboration with the molecular beam group at Perugia that extends back to Jim’s graduate school days. Later in the summer, Professors Franco Vecchiocattivi and Nadia Balucani joined Stefano.

Jim continues to work with the Kearns Center for Leadership and Diversity in Arts, Sciences and Engineering to provide academic assistance to minority students interested in pursuing careers in science. The Center is in the third year of an NSF S-STEM grant for \$598,000, for which Jim serves as PI along with Beth Olivares from the Center, to provide academic and financial assistance to STEM (Science, Technology, Engineering, Mathematics) students coming from underrepresented groups. Of particular importance for Kearns students in freshman and organic chemistry is the study group program staffed by several dedicated, talented graduate students, resulting in remarkably improved retention rates in chemistry. Jim is especially grateful to John DiMaio, Eric Henry, Jesse Kleingardner, and Megan Reesbeck for their work in general chemistry, and Peter Carlsen, Steve Jacob, and Mike Prinsell for working with students in organic chemistry.



The past year has been particularly noteworthy for Jim’s family. As we reported last year, granddaughter Josefina Emilia was born in July to daughter-in-law Mariana and son Andy in Jersey City. Fi Fi, as we call her, is now walking and talking, although we have no idea what she is saying! And last November, daughter Stacey and her husband Achim had another boy, this one named Cary Andrew, who joins big brother Callum in Manhattan. Jim and Kathy continue to make many trips to the New York City area to visit children and grandchildren.



Beloved Toby, 2003 - 2013

Rudi Fasan

Assistant Professor of Chemistry

Ph.D. 2005, University of Zürich, Switzerland



RESEARCH INTERESTS

Bioorganic chemistry and chemical biology; Synthesis and directed evolution of macrocyclic peptides and organo-peptide hybrids for molecular recognition and catalysis; Protein-protein interactions; P450 engineering and chemo-enzymatic C-H functionalization.

CONTACT

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Prof. RUDI FASAN and his group continue to be engaged in the development and investigation of novel chemobio-synthetic methodologies for the synthesis and evolution of peptide-based macrocycles to modulate protein-protein interactions and of P450-based methodologies for selective sp³ C—H functionalization. Important accomplishments in the former area include the completion of a series of systematic studies to explore the mechanism and structure-reactivity relationships for the macrocyclization of organo-peptide hybrids via an oxime-/intein thioester-mediated ligation strategy. This work, led by John Frost (forth-year graduate student) and UR undergraduate **NICHOLAS JACOB (B.S. '13)**, was published earlier this year in *Chembiochem*. Building on these studies, the same team has recently made significant progress toward implementing a method for the ribosomal synthesis of cyclopeptides inside of living bacterial cells. Complementing our methods for MOrPH synthesis, this technology is expected to provide a powerful new platform toward the discovery of bioactive, conformationally constrained peptides. Very interesting results have also been

obtained by Jessica Smith (fifth-year graduate student), who has been investigating MOrPH-based scaffolds for mimicking α -helical protein-binding motifs. In terms of new additions, the macrocycle team has expanded over the past year to include first-year graduate student Abby Cryan, who joined our Ph.D. program after graduating from Daemen College, and post-doctoral fellow Nina Bionda, who received her Ph.D. degree from Florida Atlantic University. Abby is currently setting up a system for evolving aminoacyl-tRNA synthetases for the incorporation of unnatural amino acids into proteins, while Nina is working on new methods for cyclization of ribosomally produced polypeptides.

The group members working on P450-mediated C—H functionalization have also reported important successes. **KAIDONG ZHANG'S (POSTDOC '12)** work on the development of highly regio- and stereoselective P450 catalysts for the hydroxylation of isolated sp³ C—H bonds in the antimalarial natural product artemisinin was published in the *Journal of the American Chemical Society*. To our delight, this paper

Fasan Group



was selected for a highlight in *Chemical & Engineering News* and in *JACS Spotlight*. Joshua Kolev (third-year graduate student) has been exploring the scope of this strategy by focusing on the anticancer sesquiterpene lactone parthenolide. Through remarkable work, he was able to develop selective P450 variants to enable the manipulation of two previously inaccessible aliphatic sites of this complex natural product by chemoenzymatic means. Notably, in studies conducted in collaboration with Dr. Craig Jordan at the URMC, we discovered that some of these new parthenolide derivatives exhibit improved potency and selectivity against primary leukemia cells. Based on the promising results, the group was recently awarded a three-year Translational Research Grant from the Leukemia and Lymphoma Society, which will support continuing efforts toward developing parthenolide-based drug candidates for the treatment of leukemia.

With Kaidong (sadly) leaving us to take a senior scientist position at Metaara Medical Technologies in Vancouver, the ranks of the P450 sub-group have been reinforced by the entry of two new talented postdocs, Melanie Bordeaux and Ritesh Singh. Ritesh and Melanie are currently exploring the potential of cytochrome P450s to catalyze C—H functionalization transformations beyond the canonical monooxygenation reactions. We are particularly excited about their most recent results which demonstrate the possibility to exploit these biocatalysts to catalyze (intramolecular) C—H amination reactions! While a first manuscript in this area is underway, these findings are particularly relevant to us as they open the way to an entire new area of investigation within our group.

A number of talented undergraduate students have worked on their Senior Thesis Research during the past academic year and successfully graduated in May. The group wishes best of luck to **NICHOLAS JACOB (B.S. '13)** and **PHILIP CISTRONE (BIOCHEMISTRY B.S. '13)**, who joined the Ph.D. programs in Chemistry and in Chemical Biology, re-

spectively, at The Scripps Research Institute in La Jolla, CA; to **YICK CHONG LAM (B.S. '13)**, who has started graduate studies in Chemistry at Yale University, and to **TATYANA DYNDIKOVA (B.S. '13)**, who has moved to Michigan and is currently seeking a job in industry. As the 'old guard' moves on, the group has welcomed the arrival of an enthusiastic group of new undergraduate collaborators, senior Aaron Cravens, junior Zhijie (Abe) Wu, and sophomores Christine Ziegler, Thomas Varner, and James Weitzel, who have worked in the lab during the academic year and/or summer as part of Independent Research courses and of the REU program.

Various activities and commitments contributed to make the past year a busy one for Rudi. He visited and gave invited talks at fourteen universities and colleges across the country, contributed invited lectures at the International Conference of Biomolecular Engineering, the 245th ACS National Meeting, and the American Peptide Symposium, continued to serve as grant reviewer for the National Science Foundation, and co-organized a symposium on "C—H Activation" at the 2013 American Chemical Society National Meeting in New Orleans. John Frost and Nick Jacob also traveled to New Orleans to present their research at the ACS Meeting, whereas rising senior Louis Papa embarked for a memorable trip to La Crosse, WI (24-hour trip by train due to a weather-related flight cancellation!) to attend and present his work at the 2013 National Conference of Undergraduate Research (NCUR). Finally, several members of the Fasan group participated in the 2012 ACS Northeast Regional Meeting (NERM) conveniently located in Rochester, contributing oral (Jessica Smith, Josh Kolev, John Frost) and poster presentations (Peter Krasniak, Tatyana Dyndikova, Louis Papa) about their research projects.

Last but not least, the group would like to congratulate John Frost for receiving an Elon Huntington Hooker Fellowship and Louis Papa for being awarded a highly competitive DAAD RISE fellowship, which allowed him to conduct research in a laboratory in Germany over the summer of 2013.

Fauver Stadium (Breanna Eng '13)



Chemistry Welcomes Ignacio Franco

Assistant Professor of Chemistry

Ph.D. 2007, University of Toronto



RESEARCH INTERESTS

Physical and theoretical chemistry; theory and computation as applies to dynamical processes occurring at the nanoscale.

CONTACT

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Ignacio Franco joined the Chemistry faculty at the University of Rochester in July 2013. Ignacio received his B.Sc. in chemistry from the National University of Colombia in 2001. After completing the diploma program in condensed matter physics at The Abdus Salam International Centre for Theoretical Physics in Trieste in 2002, he moved to the University of Toronto to pursue a Ph.D. in theoretical chemical physics under the guidance of Paul Brumer. Ignacio's Ph.D. work was in the field of Quantum Control and focused on investigating the use of lasers to induce ultrafast controllable currents along nanoscale junctions. In 2008 he joined Northwestern as a postdoctoral fellow in the groups of Mark A. Ratner and George C. Schatz where he worked on the theory and simulation of single-molecule pulling experiments. He then moved to Berlin to take a position as group leader and Humboldt research fellow in the Theory Department of the Fritz Haber Institute in 2011, where he investigated electronic decoherence processes in molecules.

Research in the Franco lab focuses on theory and computation as applied to dynamical processes occurring at the nanoscale. In particular, the lab uses and develops theoretical techniques that allow the identification of new methods to exert control over the behavior of matter by means of external stimuli, a topic that the group likes to refer to as "Molecules under Stress". Problems that are currently of interest in the group include: 1. Laser control of electronic properties and dynamics; 2. Electronic decoherence in molecules; 3. Theory and simulation of single-molecule pulling processes; 4. Novel spectroscopies and control in single-molecule junctions.

Selected Publications

Long-lived oscillatory incoherent electron dynamics in molecules: trans-polyacetylene oligomers, I. Franco, A. Rubio and P. Brumer, *New J. Phys.*, **2013**, 15, 043004.

Defects in DNA: Lessons from Molecular Motor Design, M. McCullagh, I. Franco, M.A. Ratner and G.C. Schatz, *J. Phys. Chem. Lett.*, **2012**, 3, 689-693.

Tunneling currents that increase with molecular elongation, I. Franco, G.C. Solomon, G.C. Schatz and M.A. Ratner, *J. Am. Chem. Soc.*, **2011**, 133, 15714-15720.

DNA-based optomechanical molecular motor, M. McCullagh, I. Franco, M.A. Ratner and G.C. Schatz, *J. Am. Chem. Soc.*, **2011**, 133, 3452-3459.

Mechanically activated molecular switch through single-molecule pulling, I. Franco, C.B. George, G.C. Solomon, G.C. Schatz and M.A. Ratner, *J. Am. Chem. Soc.*, **2011**, 133, 2242-2249.

Quantum interferences and their classical limit in laser-driven coherent control scenarios, I. Franco, M. Spanner and P. Brumer, *Chem. Phys.*, **2010**, 370, 143-150.

Single-molecule pulling and the folding of donor-acceptor oligorotaxanes: phenomenology and interpretation, I. Franco, G.C. Schatz and M.A. Ratner, *J. Chem. Phys.*, **2009**, 131, 124902.

Femtosecond dynamics and laser control of charge transport in trans-polyacetylene, I. Franco, M. Shapiro and P. Brumer, *J. Chem. Phys.*, **2008**, 128, 244905.

Minimum requirements for laser-induced symmetry breaking in quantum and classical mechanics, I. Franco and P. Brumer, *J. Phys. B*, **2008**, 41, 074003.

Robust ultrafast current in molecular wires through Stark shifts, I. Franco, M. Shapiro and P. Brumer, *Phys. Rev. Lett.*, **2007**, 99, 126802.

Laser-induced spatial symmetry breaking in quantum and classical mechanics, I. Franco and P. Brumer, *Phys. Rev. Lett.*, **2006**, 97, 040402.

Alison J. Frontier

Professor of Chemistry

Ph.D. 1999, Columbia University



RESEARCH INTERESTS

Synthetic organic chemistry; synthesis of bioactive natural products; pericyclic reactions; asymmetric catalysis; discovery of new reactions catalyzed by transition metal complexes.

CONTACT

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Professor **ALISON FRONTIER**'s research program is devoted to the planning and execution of syntheses of biologically and structurally interesting natural products. In our laboratory, the study of Nazarov cyclization began with evaluation of a new paradigm for designing precursors for Nazarov cyclization began with evaluation of a new paradigm for designing precursors for Nazarov cyclization, which led to efficient catalysis for this classic electrocyclicization. Since those early studies, we have identified alternative starting points for the cyclization. In line with this theme, this year **WILLIAM SPENCER (PH.D. '12)** spearheaded the preparation of a review article focused on 4π cationic cyclizations "Beyond the Divinyl Ketone" (see below), summarizing the recent work of our group and that of others in the field. We have also observed three different examples of rearrangement chemistry that supercede the parent cyclization pathway, and have made progress this year in understanding the factors controlling these rearrangements. Novel applications of these reactions are being developed by Steve Jacob and Yu-Wen Huang (fourth year students), who are pursuing two observations made by **JOSH BROOKS (PH.D. '12)** during his final set of PhD thesis experiments: Yu-Wen is testing chiral tertiary amine nucleophiles as catalysts for enantioselective electrocyclicization of dienyl diketones, and Steve is studying the mechanism and scope of novel cascades involving allylic acetate-containing precursors.

Our ongoing collaboration with Rich Eisenberg has become

focused on a novel type of heterogeneous gold catalyst, and its Lewis acidic reaction chemistry. Ryan Cheng (second-year student, joint with Rich) is working to characterize these mysterious gold species, which demonstrate remarkable catalytic activity in Nazarov cyclization and other cationic transformations. Peter Carlsen (fourth year graduate student), has made remarkable progress toward completing the first total synthesis of the tetrapetalone A, work that has taken us in new and exciting directions, through the challenges posed by the chemistry of a hindered, uniquely functionalized system. We are learning about the factors that impact the reactivity and diastereoselectivity of ring-closing metathesis, the synthesis and behavior of tetramic acid derivatives, and unusual oxidation pathways of congested phenol derivatives.

This year, we welcome Dan (Jessie) Wu, a graduate of UC Irvine, to the group. She is reopening our investigation of diastereoselective catalytic hydrogenation of pyrrole derivatives. We also congratulate **JOSHUA BROOKS (PH.D. '12)** and **WILLIAM SPENCER (PH.D. '12)**, who successfully defended their doctoral theses last fall. Josh is pursuing postdoctoral studies with Dr. Derek Tan at the Memorial Sloan-Kettering Cancer Center in New York City, and Bill has moved around the corner on the fourth floor to conduct postdoctoral research with Prof. Bob Boeckman. We are also pleased to report that **DANIEL CANTERBURY (PH.D. '07)** accepted a position this year in the Synthesis and Design group at Pfizer in Groton, CT.

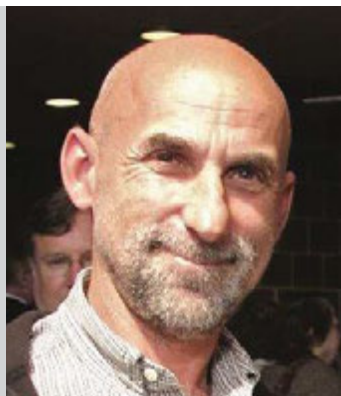


Frontier Group

Joshua L. Goodman

Professor of Chemistry

Ph.D. 1984, Yale University



RESEARCH INTERESTS

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

CONTACT

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JOSH GOODMAN's research interest is 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, they have been examining processes in which electron transfer is coupled to bond breaking, and/or bond making. These bond-coupled electron transfer (BCET) reactions have the potential to drive chemical reactions using light. They have focused primarily on dissociative return electron transfer

(DRET) reactions that involve cleavage of C-C, Si-Si and Ge-Ge bonds.

Josh serves as the Undergraduate Studies Chair and advises chemistry majors. Josh also teaches the large organic chemistry class in the fall, coupled with the smaller, Freshman Organic Chemistry course (173) in the spring.

Lightning strikes behind the River Campus (Kiera Crist '15)



Patrick L. Holland

Professor of Chemistry

Ph.D. 1997, University of California, Berkeley



RESEARCH INTERESTS

Synthetic inorganic chemistry: structure and function of models for metalloproteins, mechanisms of catalytic reactions, bioorganometallic chemistry.

CONTACT

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This is sadly the last report from **PATRICK HOLLAND**, who moved to Yale University in July of 2013. I have had a marvelous time at Rochester, both personally and professionally, and have always been impressed by the hard work and dedication of the faculty, staff, and students in the Chemistry Department. Everyone has been incredibly supportive, and I will miss you a lot. Please keep in touch!

Other than the stress of planning the move, the 2012-2013 academic year was great. We published a number of papers on low-coordinate iron in synthetic and biological scaffolds, with a special focus on spectroscopy arising from the group's growing familiarity with computational methods. These are being headed by fifth-year student Sarina Bellows, who will be staying in Rochester to finish up her Ph.D. Also staying is Zhiji Han, who has had continued great success in his joint project with Rich Eisenberg. This was highlighted by a paper in *Science* in which he teamed up with Fen Qiu (Krauss Group) to use semiconductor quantum dots to harness light for solar H₂ production. Zhiji received a prestigious Messersmith Fellowship during the upcoming year where he will finish his Rochester work.

In the fall of 2012, Pat taught General Chemistry for the first time, which was a wild ride! Grad student Nick Arnet revised the workshop problems for the course, and was an outstanding "master of demonstrations" for all three general chemistry sections. Special kudos to Nick!

Holland Group

Pat was appointed to the Editorial Board of the journal *Inorganic Chemistry*, and was elected as an upcoming chair of the Inorganic Reaction Mechanisms Gordon Conference. In the summer, he also learned that he is receiving a 2013 Blavatnik Award, which is given to young scientists in all fields in the NY/NJ/CT area. He was even interviewed for a special discussion of nitrogen fixation for a podcast from "Chemistry World" in the UK.

Alumni news abounds. **RYAN COWLEY (PH.D. '11)** and **MATT MCLAUGHLIN (PH.D. '11)** each received prestigious postdoctoral fellowships: an NIH fellowship to Ryan and an NRC fellowship to Matt. **JAVIER VELA (PH.D. '05)**, who is now a faculty member at Iowa State University, received a CAREER award from the NSF, as well as having his first child, Theodore. **JEREMY SMITH (POSTDOC '03)** is moving from New Mexico State University to Indiana University. **BEN DIBLE (POSTDOC '10)** is now doing patent research at Sanofi, and **KEYING DING (PH.D. '09)** was hired at Middle Tennessee State University. **SALLY ROCKS (PH.D. '11)** was promoted to Group Leader of the process division at FLSmidth in Utah. **CHI CHEN (M.S. '12)** and **WENWEN YAO (M.S. '12)** got married; Wenwen will be starting in Environmental Engineering at WPI in the fall of 2013, and Chi will be staying with the Holland Group at Yale for his Ph.D. Last, but certainly not least, **KAREN CHIANG (PH.D. '11)** got hitched to **ABDALLAH BITAR (M.D./PH.D. '12)**.



William D. Jones

Charles F. Houghton Professor of Chemistry

Ph.D. 1979, California Institute of Technology



RESEARCH INTERESTS

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

CONTACT

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The **BILL JONES** group continues to actively pursue organometallic chemistry and catalysis. We had four new graduate students join the group this year, Miles Marnell, Katryna Pellingra, Hongmei Yuan, and Keith Hilferding (joint with Dan Weix). Dr. Ruth Rodrigo continues as a postdoc following her Ph.D. work with Miguel Esteruelas in Zaragoza. The lab has 11 people now, and a few summer undergraduates as well. Renovations were undertaken last spring that combined rooms B42 and B46, and we now have 4 new 8-ft. hoods and a lot more instrument space! Our research is examining the activation of C-H bonds in substituted hydrocarbons, the cleavage of carbon-carbon bonds in alkynes and nitriles, and the C-S cleavage/hydrogenation of thiophenes. An important advance this year has been the elucidation of factors that control metal-carbon bond energies, such that we can now predict which products will be favored in a variety of reactions. These studies have been extended to see the effects of different ancillary ligands. 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 and new direct routes to aromatic amines from benzene. Bill continues as Associate Editor for the *Journal of the American Chemical Society* for a tenth year, where he handled close to 500 manuscripts last year. He lectured in/at Beijing, York, Brown, Scripps, Fredonia, and the GRC.

The group's scientific accomplishments have centered upon our work in alkane C-H bond activation, in which we showed that a rhodium complex first binds to an alkane and then cleaves the C-H bond. Studies have shown that the metal will only break the C-H bonds in the terminal methyl groups. Analysis of a variety of substituted hydrocarbons has now shown that alpha-electron withdrawing groups actually weaken metal-carbon bonds, not strengthen them, which appears to fly in the face of the conventional wisdom. While weaker, these bonds are not as weak as they should be (based upon the corresponding C-H bond strengths), and therefore behave as if the bond has been strengthened. Confused? Read our manuscript that appeared in *J. Am. Chem. Soc.* 2013, 135, 6994.

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 research and following the first successful three year initiation, the Center was fully funded with \$15M to support activities over a five year period, and will be up for renewal this fall. Our group is also continuing mechanistic work on C-CN cleavage. We have determined that in C-CN cleavage of benzonitriles, co-

Jones lab renovation



ordination to the arene, not the nitrile, precedes bond cleavage. Detailed DFT studies have been used to support this pathway, and a novel migratory process of the metal has been elucidated. The group continues its collaborative work on C-CN cleavage with Professor Juventino Garcia at the Universidad Nacional Autonomas de México.

Bill has also been invited back to China this fall to speak at a meeting at USTC. He will serve on the International Advisory Board for the ICOMC and the 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. We are just initiating new work with GE on liquid fuel cells.



Go Yellowjackets!

Todd D. Krauss

Professor of Chemistry and Chair

Ph.D. 1998, Cornell University



RESEARCH INTERESTS

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

CONTACT

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Lots of exciting happenings to report this year from the **TODD KRAUSS** group. First, we have two students on the cusp of graduation! Julie Smyder is close to finishing up the final drafts of her thesis and has already secured a postdoctoral research fellow position at Cornell University with UR undergraduate alum John Marohn. Helen Wei is working double duty as the mom of a new baby and writing up her thesis and she hopes to defend this fall as well.

Fen Qiu is building on the results from our work with the Eisenberg group on the production of hydrogen fuel using sunlight, nanocrystals, and inexpensive chemicals like vitamin C. Fen is making highly engineered CdSe and CdS based nanoparticles with different compositions and shapes and is testing their hydrogen generating properties. Cunming Liu, still our first and only materials science student, is using ultrafast spectroscopy to study the dynamics of electron transfer from the CdSe nanoparticles to a nickel catalyst.

Brad Loesch is still knee-deep in ultrafast optical spectroscopy and is exploring the process of generating more than one

electron per absorbed photon in carbon nanotubes. Lenore Kubie, a joint Krauss-Bren student, finished a manuscript reporting on some exciting studies of the photoinduced charge transport between heme containing proteins and carbon nanotubes. In the last few months, Amanda Preske discovered a new way to control the size of PbSe nanocrystals by changing the ligand attached to the Se during the synthesis. This method should allow her to scale up the synthesis by several orders of magnitude with no loss of nanocrystal quality! Lenore and Amanda spent three weeks in Ghana as part of the NSF IGERT Fellowship program. They visited local schools and universities and, in general, learned about the energy needs in the developing world firsthand.



Greg Pilgrim also has a manuscript ready for submission on the fabrication of vertically aligned carbon nanotube membranes, which can conduct both protons and electrons. The number of materials that can conduct an electron and proton current simultaneously can be counted on one hand so this is an exciting discovery! Nicole Briglio got the first measurements in the group of single carbon nanotube fluorescence measurements at ultracold temperatures (10 Kelvin), which was quite an accomplishment! Nicole also submitted her collaborative work with the Nilsson laboratory on using short peptides with non-natural amino acids to create suspensions of carbon nanotubes that show interesting fluorescence properties. Kelly Sowers is working on shelling CdSe quantum dots with CdS and ZnS but using secondary phosphine sulfide precursors. Kelly is most proud of her “ketchup bottle” in which she scaled up the CdSe synthesis reaction to the gram scale while creating red nanocrystals with very high fluorescence efficiencies.

The newest group members are starting to have their projects round into form as well. Zhentao Hou has had some success in making nanotube suspensions with very long nanotubes and is looking forward to studying their photophysics with high spatial resolution. Amanda Amori has successfully solubilized carbon nanotubes in fluorinated polymers and obtained high specificity in terms of solubilizing particular nanotube structures. She plans on investigating the effect of the polymer on the single nanotube photophysics. Leah Frenette has solved a major research puzzle that is as old as the initial reactions to make CdSe nanocrystals: what is the mechanism of chemical bond formation? Leah is writing up her results and we expect that this paper will garner significant attention. Finally, Jennifer Urban is our first joint Nilsson-Krauss student who is working on attaching peptides containing non-natural amino acids onto CdSe quantum dots for possible applications such as studying single molecule enzyme catalysis in vivo.

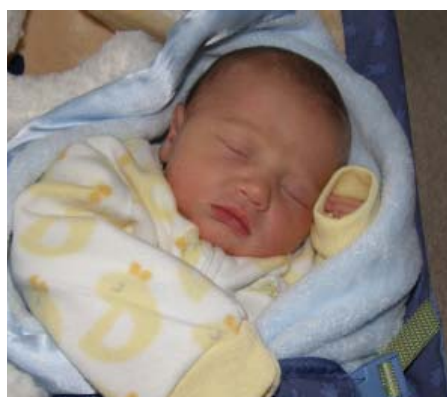
Postdoctoral fellow Dr. Michael Odoi has gotten involved in several projects in the lab. His most recent project is working to measure the “spooky” quantum mechanical nature of the photons emitted from single quantum dots as a function of laser power, a project in collaboration with Julie. Dr. Sebastian Schaefer is a new postdoctoral fellow and has gotten some exciting data on the spectroelectrochemistry properties of individual nanotubes. Preliminary data suggest that exposing the nanotubes to ambient oxygen can completely change their electrochemical response by inducing huge amounts of doping. Stay tuned as this project unfolds.

During the summer the group hosted undergraduates Chris Vela from the University of Rochester and Rebeckah Johnson

from Roberts Wesleyan College. Chris worked on solubilizing nanotubes with Zhentao and Amanda Amori while Rebeckah worked with Lenore on synthesizing heme-containing peptides to bind to nanotubes, also in collaboration with the Bren laboratory.

Todd is still in the throes of getting a new company started. He received funding from the National Science Foundation to explore ideas for possible nanocrystal based products and to train UR alum **BRETT SWARTZ (M.S. '06, PH.D. '10)** on what really matters when starting a business. We learned quickly that to customers all the fancy science behind your product matters little.

On the personal side, things were a bit crazy this spring for Todd and the family. Todd cut short his sabbatical at the ETH in Zurich to welcome Landon Matthew into the family in March (see photo). Landon remarkably sleeps 7 to 8 hours at night and we are eternally grateful for that.



Landon and Dad enjoying the annual department picnic.



Robert W. Kreilick

Professor Emeritus of Chemistry

Ph.D. 1964, Washington University



RESEARCH INTERESTS

New experimental and theoretical techniques to study molecular structure and electronic properties of transition metal complexes and paramagnetic organic molecules; and measurement of electron transfer rates between molecules held in polymers.

CONTACT

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Professor Emeritus of Chemistry, **ROBERT KREILICK's** research involved investigations of magnetic and electrical properties of solid transition metal complexes and organic free radicals. Experiments which produce information about

electron-electron exchange interactions, dipolar interactions, and electrical conductivity are conducted. New software was written for the ESR spectrometer and low temperature equipment was brought back into working order.

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

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TOM KRUGH continues his focus on support of graduate and undergraduate education and enjoys serving as an adviser to graduate and undergraduate students. In summer 2013 we had a record 35 undergraduates participating in the Research Experience for Undergraduates program that Tom has been directing since 1999. Ten students were from other schools including University of Texas at Brownsville and University of Puerto Rico Río Piedras campus. The 25 UR student par-

ticipants and 35 total undergraduates in our program reflect faculty commitment to supporting undergraduate research, which has been a Rochester tradition for many decades. Undergraduate research provides an opportunity for graduate students (and postdocs) to gain leadership experience through one-on-one mentoring that is a critical component of a successful undergraduate research experience. Mentors often describe in glowing terms their experience as mentors.



Summer REU outing

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 in photoinduced charge-transfer molecules and photoexcited nucleic acids.

CONTACT

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The **DAVE MCCAMANT** group has had a fun and productive year! This fall we welcomed Emily Hillenbrand, a first-year grad student from the University of Washington, into the group. Emily will be working on the collaborative solar hydrogen project with the Eisenberg group and this spring was accepted to the University-wide NSF Integrative Graduate Education Research and Traineeship (IGERT) program for renewable energy research. Emily will join fourth year grad student and NSF graduate research fellow, Randy Sabatini, on the Eisenberg/McCamant group collaboration that aims to combine synthesis, steady state hydrogen production and ultrafast spectroscopy to develop the first generation of solar hydrogen production cells. Randy has been collecting outstanding transient absorption spectra of a variety of chalcogeno-rhodamine dyes both free in solution and bound to TiO₂ films and has even collected femtosecond stimulated Raman spectra of these systems.

Barbara Dunlap is also now a fourth year graduate student and is continuing research into new methods for two-dimensional coherent Raman spectroscopy. Barbara's recent publication on fifth-order Raman appeared in the *John Wright festschrift* of *JPC A*. Barbara and Joohyun Lee, a third year grad student, accompanied Dave on a trip to Japan this May to attend the 2013 Time Resolved Vibrational Spectroscopy conference in Beppu. **(Side photo)** The conference was a fun opportunity to enjoy great company, science and food. At the conference, Joohyun presented his recently collected stimulated Raman spectra of dGMP, the first ever vibrational spectra of a DNA base's excited electronic state. This year we saw the departure of our fantastic postdoc, **J. REDDY CHALLA (POSTDOC '13)**, who moved to Los Angeles to be with his wife, Latha, and their brand new baby boy, Nikhil, and to start up a new postdoctoral position with Ben Schwartz at UCLA. Congratulations, Reddy! We have been very lucky to have hired a new postdoc, Collins Nganou, who joins us after getting his Ph.D. at the Technical University of Berlin, where he performed ultrafast spectroscopy on light-harvesting proteins involved in photosynthesis. Collins will be studying the ultrafast dynamics of DNA oligomers following absorption of ultraviolet light.

Throughout the year, we enjoyed working with our two senior undergraduate students, **MICAH BROWN (B.S. '13)** and **JOE COLARUOTOLO (B.S. '13)**. Micah will attend grad school

in chemistry at UNC, Chapel Hill and Joe will be attending the University of Chicago in the fall. Good job guys! We also enjoyed a year of science with Yuji Wakimoto, a junior biochemistry student, who worked on our DNA photodamage project.

We had a full house this summer, hosting two incoming first-year grad students, Dan Mark and Valerie Fleischauer, and a visiting graduate student from the University of Hong Kong, Lihong Yu. Lihong is a grad student in the lab of Prof. **DAVID PHILLIPS (POSTDOC '92)**.

Dave has had a good year, having settled into his relaxing (ha!) tenured position. He taught both CHM231 (Chemical Instrumentation lab) and CHM131-lab (General Chemistry lab) in the fall semester and was thereby able to enjoy a spring free of teaching responsibilities. He used up all of his free time to chair the graduate admissions committee though. Travelling has not been quite as busy as during the pre-tenure era, but Dave was still able to enjoy trips to Bangalore, India to attend the International Conference on Raman Spectroscopy, to Frankfurt, Germany to attend the Conference on Coherent Raman Scattering Microscopy and to Beppu, Japan to attend the Time Resolved Vibrational Spectroscopy conference.



Joohyun, Barbara, and Dave in Japan

The McCamant family is doing great, with Elise (11) moving up to 6th grade, Lydia (7) entering 3rd grade and Nora (5) starting kindergarten in the fall. Caroline is doing well having started a consulting position with GE. We're all becoming full-time dog trainers also, with the acquisition of Georgie the golden-doodle last summer.

John S. Muentzer

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

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For JOHN MUENTZER, the past year has been busy with non-academic interests: travel, family, and classical music (particularly opera) occupying much of his time. However, molecular spectroscopy is still an important part of his life. John is continuing to spend one week every couple of months working at MIT with Bob Field's group and is a co-author on a Faraday Discussions presentation. In addition, he was a co-author with MIT scientists on several papers presented at the Ohio State Molecular Spectroscopy this summer. This meeting, which

John first attended in 1963, will be the last one held at Ohio State.



Michael Neidig

Assistant Professor of Chemistry

Ph.D. 2007, Stanford University



RESEARCH INTERESTS

Physical-inorganic chemistry and catalysis: elucidation of structure and bonding in non-precious metal catalysts through inorganic spectroscopic methods; studies of reaction intermediates and mechanisms of transition metal catalysis; non-precious metal organometallic, biological and heterogeneous catalysis

CONTACT

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MICHAEL NEIDIG's group has been rapidly expanding during their second year at Rochester. The group currently consists of five Ph.D. students and has also hosted two new first year Ph.D. students this summer. We were excited to have **JARED NESVET (B.A. '13)** with us this past year before he moved on to pursue a Ph.D. in chemistry at Stanford University. Our lab facilities have expanded over the past year to now include a Mössbauer spectrometer as well as a Stopped-Flow/Rapid-Freeze Quench set-up for the elucidation of very fast kinetics and reaction intermediate identification. Our research on iron-catalyzed reactions in organic synthesis continues to

expand, including research on bisphosphine and NHC ligand systems. We have also been fortunate over the past year to establish several collaborations with leading synthetic groups around the world. As part of these collaborations, we have hosted a visiting student from Kyoto University in our group this summer. As our research progresses this upcoming year, we look forward to completing several of these studies and to continuing our foray into iron catalysis in organic synthesis.

*To the right (pg 43) -----
The Neidig Group 2012 holiday party -----*

Bradley L. Nilsson

Associate Professor of Chemistry

Ph.D. 2003, University of Wisconsin, Madison



RESEARCH INTERESTS

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

CONTACT

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The **BRAD NILSSON** group had an eventful 2012-2013. This academic year was marked by graduations, promotions, and progress in both research and teaching efforts. **NAOMI LEE (PH.D. '12)** successfully defended her Ph.D. thesis (December 2012, "Factors that Influence the Self-Assembly of Amphipathic Peptides"). Her thesis provides significant insight into the physicochemical determinants that promote self-assembly of simple amphipathic peptides. This insight will be exploited in various applications in the Nilsson group in the design of amyloid-inspired materials for biological applications. Naomi subsequently moved to Bethesda, MD where she secured a postdoctoral appointment at the National Institutes of Health (Dr. Steve Jacobson, Viral Immunology, National Institute of Neurological Disorders and Stroke). She is enjoying life in the Washington, DC area and is busy learning immunology and assisting in outreach activities at the NIH. We're thrilled with Naomi's achievements and are confident she'll leverage this excellent opportunity into even greater success.

JOHN DIMAIO (M.S. '10) and **RIA SWANEKAMP (M.S. '10)** are nearing completion of their doctoral studies. John has made significant progress on his research on the role of naturally occurring amyloid in HIV transmission processes.

In collaboration with Steve Dewhurst's group (University of Rochester Medical Center, Department of Microbiology and Immunology) he has contributed to the discovery of novel amyloid-binding agents for the detection of amyloid fibrils in semen (*Bioorg. Med. Chem. Lett.* 2013, DOI: 10.1016/j.bmcl.2013.06.097). He is also developing amyloid-inspired materials composed of self-assembled amphipathic peptides that act as microbicides for the prevention of the sexual transmission of HIV. John received an American Peptide Society Travel Grant Award to attend the 23rd American Peptide Symposium (June 22–27, 2013; Hilton Waikoloa Village, Hawaii) where he presented his research. Ria has also made significant research progress in the last year. She recently reported her discovery of the co-assembly of enantiomeric peptides into two-component hybrid fibrils (*J. Am. Chem. Soc.* 2012, 134, 5556–5559; featured in a "Spotlights on Recent JACS Publications" article *J. Am. Chem. Soc.* 2012, 134, 6057). In addition, Ria has initiated a new application for peptides developed in the Nilsson group as delivery agents for therapeutic oligonucleotides. This exciting area of research has been developed in collaboration with Dr. David Dean of the University of Rochester Medical Center. In addition to her exciting research progress, we also congratulated Ria on her marriage to **MATT BETUSH (PH.D. '13 - Boeckman group)** in 2013. John received a Moses Passer Fellowship and Ria received a Lattimore Fellowship from the Chemistry Department in recognition of their research excellence in the last year.

The other members of the Nilsson group continue to make significant strides in their research efforts as well. **WATHSALA LIYANAGE (M.S. '11)** and **ANNADA RAJBHANDARY (M.S. '13)** made key breakthroughs in their work to develop amino acid-based self-assembling hydrogel materials for tissue engineering applications. Wathsala received a travel grant award to present the results of her research at the 23rd American Peptide Symposium in Hawaii; she also received a Lattimore Fellowship from the Chemistry Department. Annada completed her M.S. studies this spring and advanced to candidacy

Neidig Group



towards the Ph.D. degree. Both Annada and Wathsala have made key discoveries regarding the self-assembly of phenylalanine derivatives applied to the creation of hydrogels for regenerative medicine. We anticipate that these discoveries will be published in the coming year. The Nilsson group also welcomed two new students in 2012-2013. Danielle Raymond and Jen Urban joined the group. They have been outstanding additions to the group and we look forward to great things from them in the future!

The Nilsson group has been fortunate to include a talented group of undergraduate students as well. **GENKI TAMIYA (B.S. '13)** conducted his senior thesis research in the Nilsson lab and will remain with the Nilsson group during the 2013-2014 academic year as he completes a fifth year towards an M.S. degree in chemistry. Annah Moore (a rising junior) has continued work on an HIV microbicide project and Kaitlyn Connelly (a rising senior) did independent research during fall 2012 and will conduct senior research in the Nilsson group this coming year. We enjoy the energy they bring to the group.

Brad has also achieved some important milestones this year. He was thrilled to be promoted to associate professor with unlimited tenure effective July 2013. He is grateful to his colleagues on the faculty and staff of the Department of Chemistry for their significant support during his time at the University of Rochester and he is excited at the prospect of

continuing these relationships for many years to come! Brad continues to serve as chair of the Harrison Howe Award Committee (Rochester Section of the American Chemical Society); he served as chair of the Travel Awards Committee for the 23rd American Peptide Symposium and he was elected as a member of the national Nominating Committee of the American Peptide Society (term of service 2013–2015). Brad taught the CHM 204 organic chemistry lecture for the first time in the Spring 2013 semester. While he has taught this material in the Quest Organic Chemistry series, the logistics of teaching a section that includes nearly 300 students was a learning experience! Brad and the Nilsson group look forward to another exciting year of research, teaching, and service.

Summer on campus



View from the Bell Tower



Oleg Prezhdo

Professor of Chemistry

Ph.D. 1997, University of Texas, Austin



RESEARCH INTERESTS

Theoretical physical chemistry with focus on dynamics in condensed phase, nanoscale and biological systems. Semiclassical theories, non-adiabatic molecular dynamics, time-dependent density functional theory, and related approaches are applied to problems in time-resolved spectroscopy, renewable energy harvesting and storage; nanoscale electronics and spintronics, and biological bonds.

CONTACT

prezhdo@chem.rochester.edu

The **OLEG PREZHDO** group has grown to its “steady-state” size of about ten people. Several group members have found academic positions: **HEATHER JAEGER (POSTDOC '13)** is starting a faculty position in the Chemistry Department at Lehigh University in Bethlehem, Pennsylvania. **TAMMIE NELSON (PH.D. '13)** obtained her doctorate and has won the prestigious Director's Postdoctoral Fellowship in Los Alamos National Lab. **RUN LONG (POSTDOC '12)** has become a Lecturer at the University College Dublin in Ireland and continues to visit the group on a regular basis. Drs. Sergiy Bubin and Lin Jun Wang have started in the group as Postdoctoral Fellows. Two new graduate students have joined the group – Jin Liu from Chemical Engineering and Dhara Trivedi from Physics. Ahmed Mustafa is finishing his tenure as a visiting scientist on a fellowship from Egypt and is getting ready to defend his Ph.D. later in the year. A recipient of a European Union exchange grant, Igor Vovchinskyi from Kharkov, Ukraine has visited the group for 4 months and has successfully defended his Master's Thesis back in the Ukraine. His advisor and long-standing collaborator, Prof. Oleg Kalugin, Chair of the Chemistry Department at the Kharkov National University, has had a month-long visit with the group. Olena Postupna is spending the summer with Dr. Sergei Tretiak in Los Alamos National Lab, gaining valuable research experience. Amanda Neukirch has won the Lindau fellowship, which has allowed her to travel to Europe and meet several Nobel Prize winners. Amanda also won a travel grant to present her research results in Japan.

Oleg Prezhdo has successfully renewed his single-PI NSF and DOE grants. The group has won a share of a collaborative grant from the Department of Energy on solar water splitting, and Dr. Alexey Akimov, Ph.D. from Rice University, is now supported by this collaboration. Japanese sci-

entists in Toyota, Inc. have approached the group to start a collaboration to study solar driven CO₂ reduction, and a postdoc in the group will be funded by Toyota for 3 years.

Over the last year, Oleg Prezhdo and his group members presented a couple dozen invited talks, published over 14 papers, including 2 reviews, a perspective, and 11 regular articles. Oleg Prezhdo organized an international workshop on “Non-adiabatic dynamics, non-equilibrium phenomena and spectroscopy” in Telluride, CO, and a Symposium on Physical Chemistry of Interfaces and Nanomaterials at the Annual Meeting of the International Society for Optical Engineering (SPIE).

Oleg Prezhdo continues to be an Editor of the *Journal of Physical Chemistry Letters* and *Journal of Physical Chemistry. The Letters* is a premier branch of *J. Phys. Chem.* with the impact factor above 6. *The Letters* is proud to report a very fast time from submission to web publication of only 40 days, compared to the 70-90 days typical of the majority of journals. Oleg's wife Marina is helping Oleg to handle the journal duties. In 2013, Oleg became an Editor for *Surface Science Reports* which publishes reviewer papers on surface science.

On a personal note, Marina runs the Russian Sunday School “Sunshine” for children aimed at maintaining the Russian culture and teaching the children the Russian language, history and arts. Marina's & Oleg's older daughter Eugenia (22) graduated Magna Cum Laude from the University of Rochester, majoring in Mathematics and minoring in Brain & Cognitive Science. She now works in a theoretical neuroscience lab in the Baylor College of Medicine. Their younger daughter Natalie (9) has finished the 3rd grade in the Mendon Center Elementary school in Pittsford. She is a regular in the Rochester Chess Club and studies ballet in the Timothy M. Draper center for Dance Education.

Lewis J. Rothberg

Professor of Chemistry

Ph.D. 1983, Harvard University



RESEARCH INTERESTS

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

CONTACT

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The **LEWIS ROTHBERG** group efforts remain primarily in organic electronics and plasmonics with occasional forays into biomolecular science and sensing. The group's funding was heavily impacted this year by the cancelation of a major three year Department of Energy grant to study plasmonic light extraction from organic light-emitting diodes (OLEDs) after the first year. Ironically, the project began to show great promise shortly after the DOE decision. We will also be feeling the effects of our valued collaborator Ching Tang moving some of his efforts to an institute in Hong Kong. He will continue to maintain a lab in Rochester for some time and we plan to work closely with his group. Lewis finally broke down and got a smart phone this year, one of the primary motivations being the OLED display and the sense it brings of the organic electronics community's accomplishments. Given Ching's enormous contributions to the invention and development of OLEDs, it has been even more inspirational to see how he continues to work hard and how dedicated he is to a deep understanding of the underlying science.

Between graduations, the discontinuation of DOE funding and students leaving for personal reasons, the group has shrunk dramatically. Our postdoctoral students **ALEX SHVEYD (POSTDOC '13)** and **IRFAN (POSTDOC '13)** took industrial employment on the West Coast while **STEVE PAQUETTE (PH.D. '13)** received his Ph.D. for work on the effects of metal nanoparticles on organic fluorescence and is now a post-doctoral student doing confocal microscopy of biomolecules. Millard Wyman is writing his thesis while Kelly Sassin and Xiao Wang chose to leave their respective doctoral programs. The remaining contingent includes Chi-Sheng Chang (plasmonic enhancement of optoelectronic devices), Ben Martin (single chain polymer spectroscopy), Chris Favaro (plasmon scattering to increase light extraction from OLEDs) and Raj Chakraborty (field effects on conjugated polymer photophysics). With group meeting so much smaller, we are especially grateful for the invigorating participation of senior scientists Al Marchetti, Ralph Young, Barbara Stwertka and William Begley who interact closely with Lewis and the students. Lewis has also enjoyed working closely with students in the Tang and Chen

Wilson Commons





Rush Rhees in the snow (Longze Zhang)

groups, Lisong Xu, Sangmin Lee, Kevin Klubek, Thomas Lee and Qiang Wang. We are also looking forward to the results of a budding collaboration with Alex Shestopalov's group in Chemical Engineering. Expect exciting developments in the lab in the year ahead!

The group has been blessed with another group of talented undergraduate researchers. **GREG MCKAY (OPTICS B.S. '13)** did an amazing senior thesis and Lewis learned a lot from him about both chemistry and optics. **DANIELLE DICKIE (B.S. '13)** also did her senior thesis on plasmonic enhancement of conjugated polymer luminescence. Thomas Bertrand, a teacher from Webster High School, developed a set of organic electronics experiments that could be done in secondary schools that leverage the excitement of our research.

Lewis taught the second semester of Physical Chemistry for advanced undergraduates (CHM 252) for the first time – what a great experience! He learned a huge amount and, if you can bear to hear him pontificate endlessly on how amazing thermodynamics and statistic mechanics are and their philosophical underpinnings, he will happily chew your ear off. Lewis brought the workshop program CHM 252 and was pleased with the results. Lewis continues to teach the advanced spec-

troscopy lab (CHM 232) with able assistance from **RAY TENG (B.S. '83, M.S. '87, M.B.A. '01)** and excellent teaching assistants.

Lewis presented work at many meetings and institutional seminars. Particularly enjoyable was the ACS meeting in New Orleans where the symposium was organized by Lewis' outstanding former graduate student Prof. **SHANLIN PAN (PH.D. '06)** who is doing excellent work at the University of Alabama. Another unusual presentation was Lewis recounting his experience with STTR grants at a small business grant forum run internally for the faculty. Thinking about that brings into focus some of the fascinating variety of experiences it is possible to have as an academician. Lewis is very grateful for those learning opportunities and he hopes that they positively impact the educational environment for students as well. In that vein, Lewis has continued his work as part time unpaid chief technical officer of Diffinity Genomics, a company originating from the group's research. Diffinity has struggled and faces another cash flow crisis in spite of the fact that sales revenues of the existing products are growing steadily and there are very promising follow-on products in development and testing. It will be a pivotal year for the company and interesting to see how the company and technology evolve.

William H. Saunders

Professor Emeritus of Chemistry

Ph.D. 1952, Northwestern University



RESEARCH INTERESTS

Physical-organic chemistry: *ab initio* and valence bond SCF calculations, proton transfer processes, mechanisms of elimination reactions, and kinetic isotope effects.

CONTACT

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The summer of 2012 included two trips to the Stratford, Ontario, Shakespeare Festival. The highlight of the visits was a one-man show by Christopher Plummer recounting how his interest in the theatre and literature developed, including some classic speeches. The fall saw more traveling, first a bicycle tour on the Eastern Shore of Maryland, with much good seafood, and then a tour of Provence in France run by the local Public TV station. I had seen a good bit of the area before, but becoming reacquainted was pleasant, as were several days in Paris at the end. I had a visit from a former student in October, John Borchardt – unhappily the last, for he died some months later. Characteristically, he was working hard on a variety of activities up to the

end. I spent Thanksgiving in Concord, NH with Anne and the granddaughters, who visited Rochester for Christmas. We did not see Claude and his wife this year. They had just moved from the Chicago area to Portland, Oregon, where Claude is working for a small software startup. The last week of March I went on another bike tour, this time in the vicinity of Williamsburg, VA. The weather was not kind: two inches of snow on the day of our arrival, though things got better later in the week. I took one day off from biking to visit the College of William and Mary, my undergraduate alma mater. Nobody from my student days (1940's) remains, but I had a nice visit with several chemistry faculty members I knew from later times.

*On January 19th, 2013, the Arnett Branch of the Rochester Public Library held a reception for the official opening of the interactive "Solar Village" demonstration display constructed and donated to the library by the **Schroeder Group** last year. The photograph shows the first visitors viewing the display and trying out some of the interactive features.*



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; non-equilibrium 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

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UDO SCHRÖDER's group has continued research in radio-chemistry and heavy-ion reaction dynamics, advanced detector development, as well as development of laser induced acceleration of ions for nuclear experiments (LIANE).

In several experiments at the LNS Catania/Italy, the group's grad students succeeded in demonstrating unexpected particle-specific capabilities of a new plastic scintillation material. The results could have important practical influences on future upgrades of the sophisticated, multi-element nuclear detection systems that provide precise imaging of complex reaction events induced by energetic heavy-ion collisions studied at accelerator laboratories around the world. The material is used in the group's new silicon multi-strip/plastic detector telescope ASTERICS.

Radio-chemical research into tritium transport has made good progress, as a series of new experiments have shown interesting trends with material and surface properties. The group's new research program has seen its first stress tests in laser induced ion acceleration and reactions induced in Li-compound targets. As expected, the intense electromagnetic fields generated in UR Omega/EP laser "shots" present an extreme environment for nuclear detection systems and interesting challenges for the experimenters. Preliminary results have already led to improved setups and laser beam pulse designs.

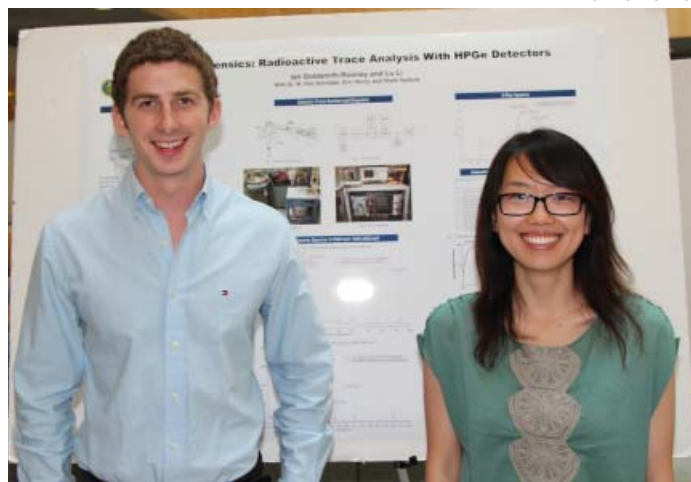
Progress has also been made on the theoretical front, in the microcanonical thermodynamic description of nuclear instabilities developing in finite nuclei at high excitations. These instabilities develop first in the nuclear surface, leading to previously unknown phenomena of surface boiling or vaporization, which explain a host of previously puzzling behavior of highly excited nuclei. Jan Töke gave a description of the theory at the International Conference of Nuclear Physics and Atomic Energy in Kyiv/Ukraine. Udo was an invited participant at the 2012 London JINA/

EMMA Workshop on Nuclear Processes in Dynamic High-Energy Density Plasmas. He also gave lectures on nuclear energy and launched an interdisciplinary course "Energy: Science, Technology & Society."

This summer's student interns, Ian Goldsmith-Rooney and Lu Li (shown below with their poster), applied nuclear forensics methods to look for trace radioactivity in construction materials from the Medical Center Annex, previously known as "Manhattan Annex". The Manhattan Project is well known as an enormous and highly successful national effort during WWII to develop the first atomic bomb. Less well known is that the project had additional aspects related to the exploration of biological effects of radioactivity, both on the battle field and in civilian medical applications. The University of Rochester Strong Memorial Hospital was one of several U.S. medical facilities that hosted one of the secret laboratories in which ethically questionable medical experiments were conducted on human subjects. These experiments have been subject to government investigations and are described in books (The Plutonium Files).

In their study, the students detected low-level residual actinide radioactivity on the concrete from one of the labs in the "Manhattan Annex." These activities are understood as traces of the secret activities conducted some 60-70 years ago.

Ian and Lu



Douglas H. Turner

Professor of Chemistry

Ph.D. 1972, Columbia University



RESEARCH INTERESTS

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

CONTACT

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The most exciting development for the **DOUG TURNER** group this year was funding of their NIH proposal. This provides resources to continue their quest to predict RNA structure from sequence, a goal becoming more and more important as sequencing of DNA and RNA gets faster and cheaper. Current estimates are that over 75% of DNA sequence in humans is transcribed into RNA. Moreover, the genomes of many viruses, including influenza, are RNA. Thus, there is a lot to be discovered. For the last few years, the group has been focusing on the roughly 10,000 nucleotides of influenza that code for proteins. Last year, **WALTER MOSS (PH.D. '11)** and his wife, Indee Dela-Moss, collaborated with **ELA KIERZEK (POSTDOC '03-05)**, Ryszard Kierzek, and **SAL PRIORE (PH.D. '13)** to provide experimental verification of the group's previously published prediction that one segment of influenza RNA folds into two different structures, potentially providing a switch that can regulate relative synthesis of two different proteins. In the fall, Walter started a postdoc with Joan Steitz at Yale. This Spring, Sal graduated and started his third year of Medical School. Doug continues as Associate Director of the MD/PhD program and is pleased to report that the NIH grant supporting it will also be renewed so that students with interests like Sal's will continue to be trained at Rochester for at least another five years.

Targeting of influenza RNA is being further advanced by the chemical mapping and NMR structural studies of graduate students **JON CHEN (OPTICS B.S. '06)**, Tian Jiang, Andy Kauffmann, and Kyle Berger. Kyle is a student in the Medical Center's Biophysics program and did his undergraduate research at SUNY Fredonia with **MATT FOUNTAIN (PH.D. '94)**. Long time collaborators from Poznan, Ela and Ryszard Kierzek, are also involved. Ela and Doug have an NIH Fogarty International Research Collaboration Award for her project. Group predictions



*Josh Blose, Ph.D., Assistant Professor at SUNY Brockport, Doug's "academic grandson" who participated in the career panel during the Chemistry-Biology-Biophysics Cluster Retreat
See pg 17*

for RNA targets are being tested in cell culture in a collaboration with Prof. Luis Martinez-Sobrido in the Department of Microbiology and Immunology. George Eastman's vision of collaboration between the College and Medical Center continues to have impact.

To provide benchmarks for testing computational approaches for predicting 3D structure, Scott Kennedy and Ryszard Kierzek published a novel structure for an internal loop. On the basis of sequence, the loop, (GAGU)₂, was expected to have two hydrogen bonded AG pairs flanked by wobble GU pairs. In fact, the major structure has two hydrogen bonded GG pairs, stacked A's, and bulged out U's. The loop also has a minor structure, which is yet to be determined. While this loop sequence has not been observed in nature, it provides another possibility for an RNA switch.

The “GAGU” loop provides an interesting case in which structure depends on the relative importance of hydrogen bonding and stacking. To provide a benchmark without hydrogen bonding, **JASON TUBBS (PH.D. '13)** collaborated with David Condon and Scott Kennedy to measure NMR spectra of CCCC and compare the results to molecular dynamics calculations using a standard force field and a new one developed at Rochester by **ILYAS YILDIRIM (PHYSICS PH.D. '08)**. The new force field is clearly better. The results also provide insight into experiments from **PHIL BEVILAQUA'S (PH.D. '93)** lab showing that hairpin loops of C4 are less stable than those of U4. Jason graduated and took a position at SynDaver Labs in Tampa.

While the current approximations in force fields do not allow agreement between predictions and experiment, the theoretical groups of Morgado in Chile and Sponer in the Czech Republic published a paper reporting that quantum mechanics calculations can reproduce aspects of how the structure formed by tandem GA pairs depends on stacking with the adjacent base pairs, as determined with NMR by **JOHN SANTALUCIA (PH.D. '91)**, **MING WU (PH.D. '96)**, and **GANG CHEN (PH.D. '05)**. Thus, there is hope that known physical principles will eventually be able to predict the 3D structures of RNA sequences.

Turner Group

Doug presented the group's work at Alnylam Pharmaceuticals, the annual meeting of the Oligonucleotide Therapeutics Society, Konan University in Kobe, the 39th International Symposium on Nucleic Acid Chemistry held at Nagoya University, and at the Institute for Bioscience & Biotechnology Research at the University of Maryland. At all these venues, Doug was impressed by the increased prospects for development of therapeutics targeting RNA. Another indication is that in recognition of his work on discovering potential drugs for RNA, **MATT DISNEY (PH.D. '02)** was named the winner of the American Chemical Society 2013 Eli Lilly Award in Biological Chemistry.

Doug taught a section of the Spring General Chemistry course and also part of the graduate Biophysical Chemistry course. The latter was shared with **DAVE MATHEWS (PH.D. '01)** and Alan Grossfield from the Medical Center's Department of Biochemistry and Biophysics. This provides another example of the impact of George Eastman's vision. Doug also did research with undergraduate **ULASCAN SARICA (PHYSICS B.S. '13)** and supervised the research of **JAYSON BAMAN (BIOLOGY B.S. '13)** in collaboration with Sal Priore. Ulaskan is entering the graduate program in Physics at Johns Hopkins University and Jayson will be a first year medical student here.



Daniel J. Weix

Assistant Professor of Chemistry

Ph.D. 2005, University of California, Berkeley



RESEARCH INTERESTS

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

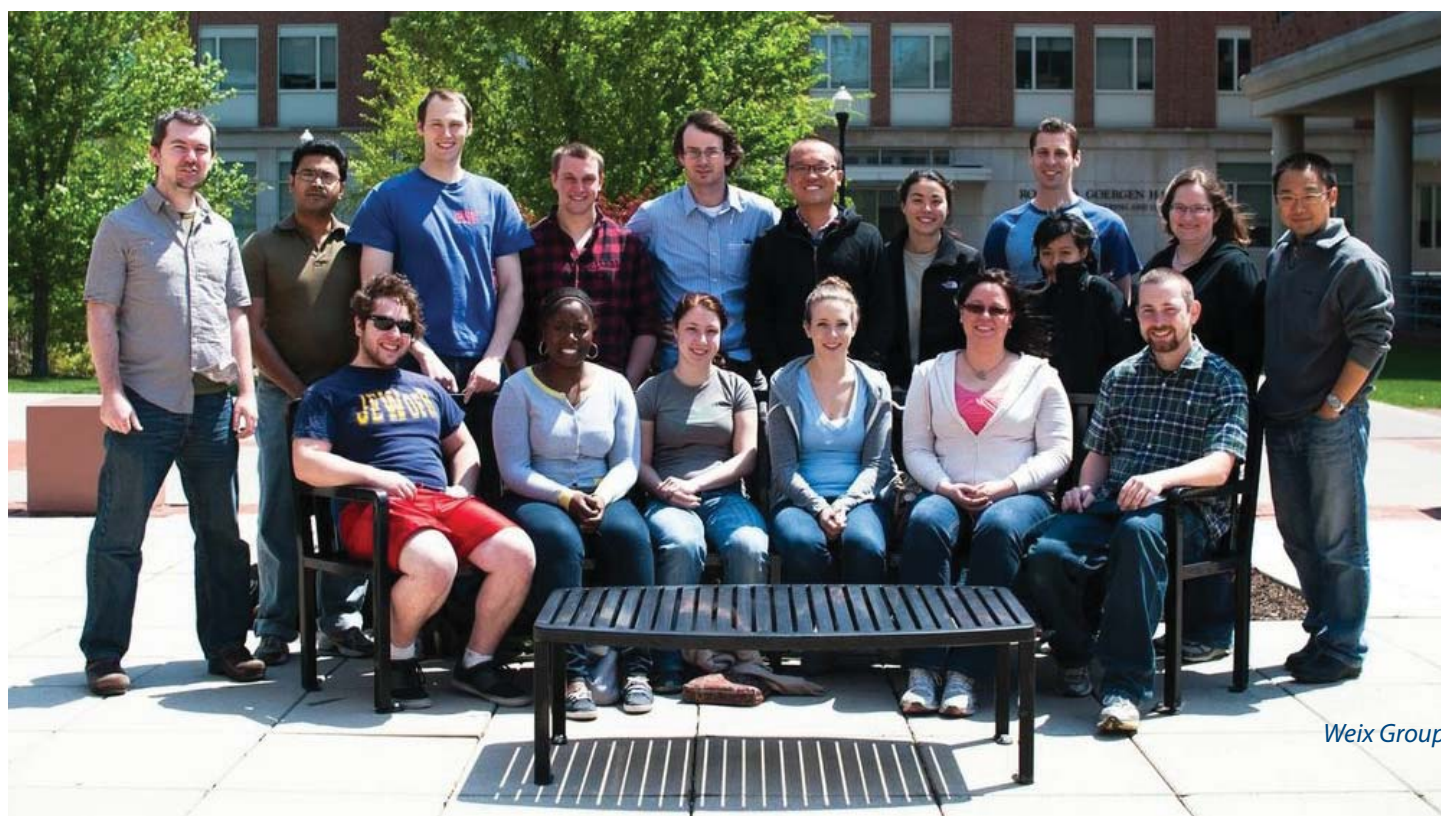
CONTACT

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Research in **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. We have continued to advance the practice and theory of "cross-electrophile coupling" as an alternative to the usual cross-coupling of a nucleophile with an electrophile. Because this chemistry avoids the need to pre-form carbon nucleophiles, it has attracted broad interest and is under active investigation or use at most major pharmaceutical companies. By leveraging our recent advances in mechanistic understanding, we have embarked on the development of "2nd-generation" systems that utilize new electrophiles and often feature multiple catalysts. Michael Prinsell and Lukiana Anka-Lufford's full-paper on coupling allylic acetates with alkyl, vinyl, and aryl halides was published in the *Journal of Organic Chemistry* this past fall. **RUJA SHRESTHA (PH.D. '12)** and Stephanie Dorn published their full paper on the reductive conjugate addition of aryl halides to enones in the *Journal of the*

American Chemical Society. Finally, **DANIEL EVERSON (PH.D. '13)** and **DAVID GEORGE (B.S. '13)** published a large-scale procedure for the alkylation of aryl halides with alkyl halides in *Organic Syntheses*. Chi Chen, a joint student between the Weix and Holland groups, has developed the first Z-selective isomerization of simple alkenes using one of the Holland group's tri-coordinate cobalt diketimines. This has been a productive year and the manuscripts are piling up on Daniel's desk! In the next few months we will submit manuscripts on the mechanism of cross-electrophile coupling, new types of electrophiles, carbonylation, multimetallic chemistry, olefin isomerization, reactions of heterocycles and several reviews.

The group was fortunate to be recognized with a variety of awards and honors this past year. **ADAM LEE (B.S. '12)** was awarded a Jamaica 50th Anniversary Scholarship which will defray the cost of his medical training at the University of the West Indies. **RUJA SHRESTHA (PH.D. '12)** thesis



was selected for commendation by the Outstanding Dissertation Awards program in AS&E. **DAVID GEORGE (B.S. '13)** won the UR Research Expo President's Award. **RACHEL KELEMEN (B.S. '12)** received a Chemistry Department Award at Graduation. Third-year Lukiana Anka-Lufford was selected for a 1-year co-op with the GlaxoSmithKline Anti-Bacterial team. Luki left for King of Prussia, PA in May and will return next spring to inform us all about how things are really done in industry! Finally, Daniel Weix received a number of awards on behalf of the entire Weix group: a Green Chemistry Award from the Pfizer-Groton Green Chemistry Team (2012), a Thieme Journal Prize (2013), and a Sloan Foundation Fellowship (2013).



Earlier this year, we welcomed three new graduate students: Sylvia Chen, Keith Hilferding, and Kierra Huihui. Keith is a joint student between the Jones group and the Weix group and will be studying oxidative addition reactions of nickel(0) to various electrophiles. Kierra has already worked out a new type of conjugate-addition-like reaction and Sylvia has spent her time working on several new directions for the group. We also welcomed 3 new undergraduate researchers: seniors Michael Robo and Matt Lovell ('14), and sophomore Charlotte Humes. The group now has 12 full-time researchers plus 4 active undergraduates after a peak of 19 researchers this past summer. Finding a large enough room for meetings became a challenge!

In May, we celebrated the graduation of five current and former group members. **JOSEPH BUONOMO (B.S. '13)**, **DAVID GEORGE (B.S. '13)**, and **RACHEL KELEMEN (B.S. '13)** graduated and are moving on to graduate school at the University of Minnesota, the University of California, Irvine, and Boston College, respectively. We look forward to reading their work in future issues of *JACS*! **MAX HECHT (B.S. '13)** graduated after finishing his senior thesis working on a Holland/Weix joint project with Chi Chen, but he started in the Weix group working with Dan Everson. Max is moving

on to brewmaster school and we look forward to drinking his future work. **DANIEL A. EVERSON (PH.D. '13)**, who mentored Joe, David, and Max, defended his thesis in May. He has relocated to Minneapolis, MN where he will enjoy some time off with his wife, Kelsey, and new daughter, Cora, before finding employment in the metro area. Daniel will not easily be replaced and will be greatly missed.

Besides their excellent results in the laboratory, third-year students Lukiana Anka-Lufford, Chi Chen, Stephanie Dorn, and Laura Ackerman all passed their oral exams in style. Lukiana, Stephanie, and Laura also each successfully delivered a third-year talk on an outside topic to the department. Laura Ackerman was a class-leader for the Horizons summer program at the University of Rochester last summer. She guided a group of middle-school students through some fun chemistry experiments with the goal of bringing students from under-represented backgrounds into the sciences. **DANIEL A. EVERSON (PH.D. '13)** and his wife Kelsey welcomed their first child, Cora, into the world last fall and Chi married Wenwen this spring at the beautiful Letchworth state park in front of a waterfall. Chi Chen moved to Yale University with Prof. Holland's group this summer, but will remain a joint student. Daniel Weix's children, Elliott (8), Madeleine (6), and Amalia (4), continue to keep him and his wife, Stella, busy.

In group alumni news, **BRITTANY JONES (B.S. '11)** is currently working at Materia, the L.A.-based ruthenium olefin metathesis catalyst company, and enjoying the varied opportunities available at the smaller-sized company. **RUJA SHRESTHA (PH.D. '12)** is off to a great start in her postdoc with John F. Hartwig. She just published her first paper there on sterically-directed C-H amination in *J. Am. Chem. Soc.*



Publications '12-'13

Includes publications accepted or submitted between July 2012 and June 2013.

ROBERT K. BOECKMAN, JR.

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JOSEPH P. DINNOCENZO

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SAMIR FARID

Chain Amplified Photochemical Fragmentation of N Alkoxyridinium Salts: Proposed Reaction of Alkoxy Radicals with Pyridine Bases to Give Pyridinyl Radicals. D. Shukla, S. Adiga, W. Ahearn, J. P. Dinnocenzo, S. Farid, *J. Org. Chem.*, **2013**, 78, 1955-1964.

JAMES M. FARRAR

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RUDI FASAN

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ALISON J. FRONTIER

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PATRICK L. HOLLAND

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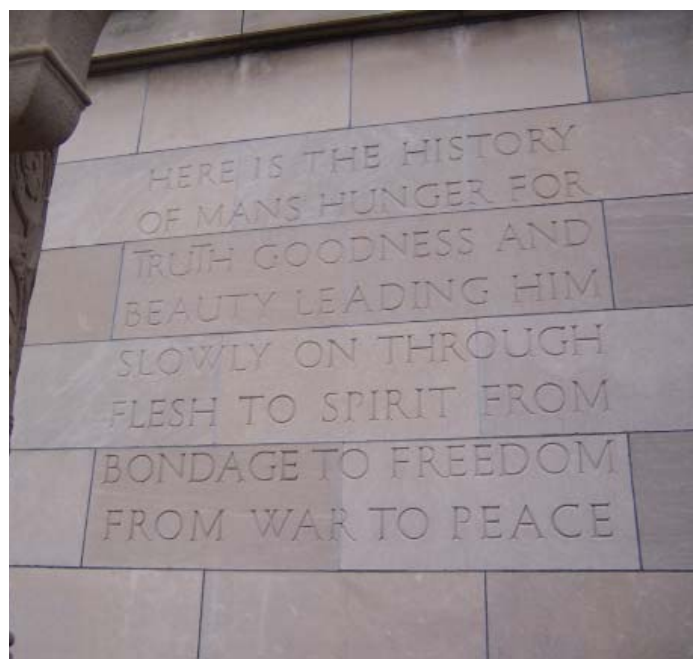
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WILLIAM D. JONES

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TODD D. KRAUSS

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DAVID W. MCCAMANT

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JOHN S. MUENTER

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MICHAEL L. NEIDIG

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BRADLEY L. NILSSON

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OLEG PREZHDO

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LEWIS J. ROTHBERG

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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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Chemistry/Biology Undergraduate Poster Session at Open House



Fellows 12-'13

Ahmed Mohamed Mustafa Abuella

Visiting Graduate Student
Al-Azhar University, Egypt, 2013

Albert Collins Nganou Assonkeng

Technical University, Berlin, Germany 2012

Nina Bionda

Florida Atlantic University, USA, 2013

Soumik Biswas

State University of New Jersey - Rutgers, USA,
2010

Melanie Bordeaux

l'Ecole Nationale Supérieure de Chimie de
Montpellier (ENSCM), France, 2012

Sergiy Bubin

University of Arizona, USA, 2006

Jagannadha (Reddy) Challa

Case Western Reserve University, Cleveland,
OH; Indian Institute of Technology, Madras,
India, 2007

Amit Das

Indian Institute of Technology, Bombay, India,
2012

Yuming Dong

Nanjing University, China, 2008

William Eckenhoff

Duquesne University, Pennsylvania, USA, 2010

Katarzyna Grubel

Utah State University, USA, 2011

Irfan

University of Rochester, New York, USA, 2012

Heather Jaeger

University of Georgia, USA, 2010

Run Long

Shandong University, P.R. China, 2008

Kenneth ("Cory") MacLeod

University of British Columbia, Okanagan,
Canada, 2012

Michael Odoi

University of Massachusetts, USA, 2010

Linsen Pei

University of Science and Technology of
China, P.R. China, 1999

Ruth Castro Rodrigo

University of Zaragoza, Spain, 2010

Marie-Pierre Santoni

Université de Montréal, Canada, 2010

Sebastian Schaefer

University of Siegen, Germany, 2008

Alexander Shveyd

Northwestern University, Illinois, USA, 2011

Ritesh Singh

University of Lucknow, India 2007

William Spencer

University of Rochester, New York, USA, 2012

Brett Swartz

University of Rochester, New York, USA, 2010

Francesca Vitali

Universität Zürich, Switzerland; La Sapienza-
Università di Roma, Italy, 2003

Guiqing Zhang

Visiting Postdoc
Shandong University, P.R. China, 2007



Commencement

Bachelors and Masters Degrees Awarded in Chemistry

2013 BACHELOR OF SCIENCE

Micah Brown^{3†}
Nathaniel Brown, Jr.^{3†}
Joseph Buonomo
Melissa Cardona
Joseph Colaruotolo³
Cole Cruz¹
Brandon Daehn
Benjamin Dick
Danielle Dickie
Tatyana Dyndikova
David George¹
Alison Hamlin^{3†}
Maxwell Hecht
Nicholas Jacob²

Rachel Kelemen³
Hoon Kim
Yick Chong Lam³
Joanne Leadbetter
Carina Luck²
Taylor Moot¹
Mikael Olezeski^{2**}
Anish Patel¹
Jessamyn Perlmutter^{2**}
Ian Pershing^{**}
Adbel Reyes^{*}
Melissa Scharoff
Genki Tamiya
Lidong Wang
Jessica Weber

2013 MASTER OF SCIENCE

Malik Al-Afyouni
Nicholas Arnet
Jill Caputo
Ryan Cheng
Stephanie Daifuku
Stephanie Dorn
Adam Feinberg
Zhentao Hou
Banu Kandemir
Andrew Kauffmann

Jared Kneebone
Lloyd Munjanja
Olena Postupna
Annada Rajbhandary
Megan Reesbeck
Gilbert Reynders
Rebecca Smith
James Virnelli III
Yang Zhao

DISTINCTIONS

¹Distinction

²High Distinction

³Highest Distinction

*Take 5 Scholar (finishing)

**Take 5 Scholar (beginning)

†Phi Beta Kappa

2013 BACHELOR OF ARTS

Chandra Ade-Browne^{**}
Joshua Bielemeier²
Shane Borzok^{2**}
Brittany Bratek
Breanna Eng¹

Joshua Geiger^{3**}
Tyler Gomez-Basauri
Benjamin Hyers^{3†}
Samina Aleen Khan^{*}
Corinne Land

Jendayi Mack
Sonia Mandal
Matthew Metz
Kaitlyn Mokay
Jared Nesvet^{3†}

Kaitlin Marie Pellicano
Zachary Pressman²
Shaun Sheikh
Luxi Shen
David Shin¹
Emily Wyckoff

2013 Chemistry Graduates



Doctoral Degrees Awarded in Chemistry

Joshua Brooks

Synthetic Studies of Reaction Cascades Initiated by 1,6-Conjugate Addition
Alison Frontier

Jennifer Ciesielski

I. *Introduction to Phomactin A*
II. *The B-Iodoallenolate Cyclization,*
III. *Studies Toward the Synthesis of Phomactin A*
Alison Frontier

Naomi Lee

Factors that Influence the Self-Assembly of Amphipathic Peptides
Bradley Nilsson

Tammie Nelson

Nonadiabatic Excited State Molecular Dynamics: Perspectives for a Robust Future
Oleg V. Prezhdo

Leslie Ofori

Solving the Problem of RNA Sequence Selectivity by Small Molecules with Application to Myotonic Dystrophy Type 1 and HIV-1
Benjamin Miller

Steve Paquette

Enhanced Photostability In Organic Thin Films Deposited On Plasmonic Substrates
Lewis Rothberg

Salvatore Priore

Discovery and Characterization of Influenza Virus RNA Secondary Structures
Douglas Turner

Meghan Rodriguez

Studies of B-Diketiminato Iron Complexes to Investigate Nitrogen Activation and Novel Iron-Sulfur Clusters
Patrick L. Holland

William Spencer

The Development of Cyclization Reactions Engendered by Synthetic Studies Toward Rocaglamide
Alison Frontier

Tulaza Vaidya

Electrophilicity-driven Annulations of Polarized Nazarov Precursors with Tricationic Iridium(III) and Heterogeneous Gold Catalysts
Richard Eisenberg/Alison Frontier

2013 Chemistry Faculty



Student Awards

DEPARTMENT AWARDS

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

John McCreary Memorial Prize
Nathaniel Brown, Jr.

ACS Rochester Section Award
Joseph Colaruotolo

ACS Inorganic Chemistry Award
Luxi Shen

ACS Organic Chemistry Award
Jared Nesvet

Chemistry Department Award
Joshua Bielemeier
Alison Hamlin
Benjamin Hyers
Nicholas Jacob
Rachel Kelemen
Zachary Pressman

**CRC Press Chemistry Achievement Award
for Senior**
Yick Chong Lam

Distinguished Service Award
Breanna Eng

COLLEGE AWARDS

Janet Howell Clark Prize
Alison Hamlin

Catherine Block Memorial Fund Prize
Hee Young (Rachel) Park

**Edward Peck Curtis Award for Excellence
in Teaching by a Graduate Student**
Kimberly Manbeck



Student Awards

TEACHING AWARDS

W. D. Walters Teaching Award

Adam Feinberg, Jeffrey Kehl, Jared Kneebone,
Gilbert Reynders, James Virnelli

Carl A. Whiteman, Jr. Teaching Award

Nathaniel Brown, Jr., Benjamin Hyers

ENDOWED DEPARTMENT FELLOWSHIPS

Robert and Marian Flaherty DeRight Fellowship

Jonathan Chen, Peter Carlsen

Moses Passer Fellowship

John DiMaio

Elon Huntington Hooker Fellowship

Zhiji Han, Eric Henry, Salvatore Priore,
Jessica Smith

Arnold Weissberger Fellowship

Joshua Brooks, John Frost, Yunzhe Jiao,
Yeketerina Lyubarskaya, Michael Prinsell,
William Spencer, Alexander Wotal

Samuel Allen and Ellen Frances Lattimore Fellowship

Nicole Briglio, Wathsala G. H. M. Liyanage,
Ria Swanekamp

Robert L. & Mary L. Sproull Fellowship

Jennifer Urban

PHI BETA KAPPA

Micah Brown, Nathaniel Brown, Jr., Alison
Hamlin, Benjamin Hyers, Jared Nesvet



JULY 2012

Professor Thomas Ward (University of Basel, Switzerland) *"Artificial Metalloenzymes: Merging the Best of Homogeneous and Enzymatic Catalysis,"* July 23, 2012

Nicole Briglio (University of Rochester) *"Photophysics of Isolated Single-Walled Carbon Nanotubes,"* July 23, 2012

Meghan Marguerite Rodriguez (University of Rochester) *"Studies of B-Diketiminato Iron Complexes to Investigate Nitrogen Activation and Novel Iron-Sulfur Clusters,"* July 27, 2012

AUGUST 2012

Leslie Odame Ofori (University of Rochester) *"Solving the Problem of RNA Sequence Selectivity by Small Molecules with Application to Myotonic Dystrophy Type 1 and HIV-1,"* August 6, 2012

Professor Young Kuk (Seoul National University) *"Edge States in a Graphene and Defect States in Quantum Dots Studied with Low-Temperature Scanning Probe Microscopy,"* August 17, 2012

SEPTEMBER 2012

Professor Christine Thomas (Brandeis University) *"Metal-Metal Multiple Bonds In Early/Late Heterobimetallics: Small Molecule Activation and Catalytic Applications,"* September 17, 2012

William Spencer (University of Rochester) *"The Development of Cyclization Reactions Engendered by Synthetic Studies Toward Rocaglamide,"* September 20, 2012

Professor Matthew Francis (University of California, Berkeley) *"Building New Materials Using Synthetically Modified Biomolecules,"* September 21, 2012

Professor Curtis Berlinguette (University of Calgary, Canada) *"Extending the Warranty of the Dye-Sensitized Solar Cell,"* September 24, 2012

OCTOBER 2011

Harrison Howe Award Lecture

Professor Xiaoliang Sunney Xie (Harvard University) *"The Quest for Non Linear Coherent Optical Imaging for Biology and Medicine,"* October 2, 2012

Professor Xiaoliang Sunney Xie (Harvard University) *"Life at the Single Molecule Level,"* October 2, 2012

Professor Daniel Romo (Texas A&M University) *"Bioactive Natural Products: Synthetic Studies Fueling Discoveries at the Chemistry-Biology Interface,"* October 3, 2012

Dr. Jay A. Labinger (California Institute of Technology) *"Going with the Flow: Mechanistic Studies on the Selective Catalytic Conversion of Methanol/Dimethyl Ether to Triptane,"* October 5, 2012

Seymour Rothchild Lecture

Dr. Matthew C. Beard (Center for Advanced Solar Photophysics, Chemical and Material Sciences Center, National Renewable Energy Laboratory) *"Progress Towards Third Generation Solar Energy Conversion: Can Quantum Dot Solar Cells Exceed the Shockley-Queisser Limit?"* October 10, 2012

Professor Ulrich Wiesner (Cornell University) *"Cornell Dots: From Fundamentals of Fluorescent Silica Nanoparticles to Translational Clinical Applications,"* October 17, 2012

Professor Xiaoyang Zhu (University of Texas at Austin) *"Solar Energy Conversion Beyond the Limit,"* October 22, 2012

Professor Bradley Nilsson (University of Rochester) *"Peptide Self-Assembly: From Pathological Amyloid to Engineered Biomaterials,"* October 24, 2012

NOVEMBER 2012

Professor Esther Conwell (University of Rochester) “*Conductance of DNA*,” November 7, 2012

Joshua L. Brooks (University of Rochester) “*Synthetic Studies of Reaction Cascades Initiated by 1,6-Conjugate Addition*,” November 9, 2012

Professor Marcetta Darensbourg (Texas A&M University) “*Molecular Constructs as [FeFe]-H₂ase Enzyme Active Site Biomimetics for Proton Reduction*,” November 12, 2012

Professor Christopher C. Cummins (Massachusetts Institute of Technology) “*Chemistry in Confinement*,” November 14, 2012

Professor Hitomi Mukaibo (University of Rochester) “*Microneedle-Array Based Gene Delivery for Microalgae Cells*,” November 28, 2012

Professor Alex Shestopalov (University of Rochester) “*Functional and Structured Hybrid Material Interfaces*,” November 28, 2012

Professor Christopher Vanderwal (University of California at Irvine) “*Studies on Complex Natural Products*,” November 30, 2012

DECEMBER 2012

Felipe Angel (University of Rochester) “*Novel Approaches to Increase the efficiency of Polymer-based Organic Photovoltaic Devices*,” December 3, 2012

Dr. Scott D. Edmondson (Merck & Co. Inc.) “*Discovery of JANUVLA™ (Sitagliptin): A Selective Dipeptidyl Peptidase 4 Inhibitor for the Treatment of Type 2 Diabetes*,” December 7, 2012

Professor Nilay Hazari (Yale University) “*Common Mechanisms for Carbon Dioxide Activation and Organic Transformations*,” December 10, 2012

Professor Stephen W. Ragsdale (University of Michigan Medical School) “*Regulation of Protein Function by Heme, Redox, and CO*,” December 12, 2012

Tammie Nelson (University of Rochester) “*Nonadiabatic Excited State Molecular Dynamics: Energy Transfer in Conjugated Polymers*,” December 17, 2012

Naomi Lee (University of Rochester) “*Factors that Influence the Self-Assembly of Amphipathic Peptides*,” December 18, 2012

JANUARY 2013

Dr. Heather Jaeger (University of Rochester) “*Effective Solar Energy Conversion from Nanoscale Photovoltaics*,” January 7, 2013

Gregory Pilgrim (University of Rochester) “*Fabrication and Characterization of Carbon Nanotube Membranes for Hydrogen Production Applications*,” January 11, 2013

Professor Zachary Schultz (University of Notre Dame) “*Nanostructures for Label-Free Detection and Imaging*,” January 14, 2013

Professor Scott Phillips (Pennsylvania State University) “*New Strategies in Reagent Design for Point-of-Use Diagnostics*,” January 18, 2013

Professor Theodore Betley (Harvard University) “*Correlation of Electronic Structure to Reactivity in Organometallic Catalysis and Polynuclear Small Molecule Activation*,” January 21, 2013

Professor Chris Douglas (University of Minnesota, Twin Cities) “*Transition Metal Catalysis with Sigma Bonds to Carbon Adjacent to Carbonyls*,” January 25, 2013

Professor Robin Bedford (University of Bristol, UK) “*Iron Cauldrons and Witches’ Brews*,” January 28, 2013

FEBRUARY 2013

Professor Giovanna Ghirlanda (Arizona State University) “*De Novo Design of Functional Protein Assemblies: Towards Hydrogen Production*,” February 1, 2013

Professor Chaim N. Sukenik (Bar Ilan University) “*Controlling the Reactivity, Stability and Stiffness of Interfaces using Self-Assembled Monolayers and Thin Oxide Films*,” February 4, 2013

Steve Paquette (University of Rochester) “*Enhanced Photostability In Organic Thin Films Deposited On Plasmonic Substrates*,” February 7, 2013

Professor Alex Deiters (North Carolina State University) *"Synthetic Chemical Tools for the Regulation of Cellular Processes,"* February 8, 2013

Victor J. Chambers Memorial Lecture

Professor Herbert Waldmann (Max Planck Institute of Molecular Physiology) *"Biology Oriented Synthesis,"* February 11, 2013

Professor Herbert Waldmann (Max Planck Institute of Molecular Physiology) *"Hunting the Targets of Natural Product Inspired Compounds,"* February 12, 2013

Professor Herbert Waldmann (Max Planck Institute of Molecular Physiology) *"Small Molecule Inhibition of Ras Signaling – A System's Approach,"* February 13, 2013

Joshua Kolev (University of Rochester) *"Selective Aliphatic C-H bond Activation via Iron-Based Catalysts,"* February 15, 2013

Dr. David L. Clark (Los Alamos National Laboratory) *"Covalency and the Relative Roles of 5f and 6d Orbitals in Actinide Metal-Ligand Bonds,"* February 18, 2013

Professor Sarah Reisman (California Institute of Technology) *"New Methods and Strategies for the Enantioselective Synthesis of Polycyclic Natural Products,"* February 22, 2013

MARCH 2013

Kyle Biegasiewicz (University of Rochester) *"Recent Mechanistic Insight into the Stereoselective Conjugate Addition of Aldehydes to Nitro-olefins Catalyzed by Diarylprolinol Silyl Ethers,"* March 1, 2013

Professor Jason McNeill (Clemson University) *"Nanoscale Imaging with Conjugated Polymer Nanoparticles,"* March 4, 2013

Douglas Tusch (University of Rochester) *"Mechanistic Investigation of the Oxidative Mannich Reaction with tert-Butyl Hydroperoxide,"* March 15, 2013

Andrew S. Kende Distinguished Lecture

Professor Darren J. Dixon (University of Oxford, UK) *"Enantioselective Cooperative Catalysis With and Without Metals,"* March 11, 2013

Professor Darren J. Dixon (University of Oxford, UK) *"Catalyst Control in Complexity Building Reaction Cascades,"* March 12, 2013

Professor Darren J. Dixon (University of Oxford, UK) *"The Battle of Nakadomarin A and other Campaigns in Complex Natural Product Synthesis,"* March 13, 2013

Professor Theodor Agapie (California Institute of Technology) *"Heterometallic Models of the Oxygen Evolving Complex of Photosystem II,"* March 18, 2013

Professor Teri Odom (Northwestern University) *"Gold Nanostars as Tiny Hitchhikers for Cancer Therapeutics,"* March 20, 2013

Professor Eric Ferreira (Colorado State University) *"Accessing and Harnessing Metalated Intermediates Toward Synthetic Utility,"* March 22, 2013

Laura Ackerman (University of Rochester) *"Advances in C-N Bond Formation: Using Co(II) Porphyrin Catalysts for Nitrene Transfer Reactions,"* March 25, 2013

Jason Daniel Tubbs (University of Rochester) *"Computational and Experimental Advances in the RNA Therapeutic Pipeline,"* March 27, 2013

Lukiana Anka-Lufford (University of Rochester) *"Mechanistic Investigation of the Gold-Catalyzed Cyclization of Monoallylic Diols,"* March 29, 2013

APRIL 2013

Professor Timothy M. Korter (Syracuse University) *"Terahertz Spectroscopy of Crystalline Pharmaceuticals,"* April 1, 2013

Tammie Nelson (University of Rochester) *"Nonadiabatic Excited State Molecular Dynamics: Perspectives for a Robust Future,"* April 2, 2013

Dr. Sergei Tretiak (Los Alamos National Laboratory) *"Localization of Electronic Excitation in Organic Semiconductors: Theoretical Views from Different Angles,"* April 3, 2013

Stephanie Dorn (University of Rochester) *"Mechanistic Insight into the Cu(I) and TEMPO Catalyzed Oxidation of Alcohols,"* April 12, 2013

Salvatore Fortunato Priore, Jr. (University of Rochester) *"Discovery and Characterization of Influenza Virus RNA Secondary Structures,"* April 12, 2013

Professor Marcey Waters (University of North Carolina, Chapel Hill) *"Designing Molecules for Biomolecular Recognition,"* April 22, 2013

Charles F. Hutchison Memorial Lecture

Professor David Milstein (The Weizmann Institute of Science) *"Discovery of Sustainable Catalytic Reactions for Synthesis,"* April 22, 2013

Professor David Milstein (The Weizmann Institute of Science) *"Pincer Complexes: Bond Activation, Catalysis and Unusual Structures,"* April 23, 2013

Professor David Milstein (The Weizmann Institute of Science) *"Water Activation by Metal Complexes,"* April 24, 2013

Professor Carlos Simmerling (SUNY - Stony Brook) *"Using Computer Simulations to Investigate Dynamic Aspects of Inhibitor Binding and Potency,"* April 24, 2013

Professor Jonathan Owen (Columbia University) *"The Coordination Chemistry of Cadmium Chalcogenide Nanocrystals,"* April 29, 2013

MAY 2013

Professor Mitch Anthamatten (University of Rochester) *"Engineering Ion-Conductive Soft Materials for Energy Applications,"* May 6, 2013

Professor Jianshu Cao (Massachusetts Institute of Technology) *"Quantum coherence in energy transfer systems,"* May 8, 2013

Professor Vincent Gandon (Université Paris-sud, Institut de Chimie Moléculaire et des Matériaux d'Orsay - ICMMO) *"Practical Homogeneous Au(I)- and Ga(III)-Catalysis: a Few Tips,"* May 10, 2013

Olena Postupna (University of Rochester) *"Photo-induced energy transfer in carbon nanotube aggregates,"* May 13, 2013

Annada Rajbhandary (University of Rochester) *"Improving Tumor Specificity in Chemotherapy,"* May 17, 2013

Zhiji Han (University of Rochester) *"Catalytic Water Oxidation for O₂ Evolution,"* May 20, 2013

Daniel A. Everson (University of Rochester) *"Nickel-Catalyzed Electrophile Cross-coupling of Aryl Halides with Alkyl Halides,"* May 30, 2013

Nanomaterials Symposium

Frontiers in Materials Science for the 21st Century- Novel Materials for Sustainable Catalysis

Professor Shouheng Sun (Brown University) *"Rational Synthesis of Metallic Nanoparticles for Catalytic Applications"* May 20, 2013

Professor Robert M. Rioux (The Pennsylvania State University) *"Prediction and Design of Materials from Crystal Structures to Nanocrystal Morphology and Assembly,"* May 20, 2013

Professor Peng Chen (Cornell University) *"Single-nanoparticle catalysis at single-turnover and nanometer resolution"* May 20, 2013

Dr. James T. Muckerman (Brookhaven National Laboratory) *"Photocatalytic water oxidation at the GaN (1010) – water interface,"* May 20, 2013

Alexander Shestopalov (University of Rochester) *"Stable and functional hybrid interfaces via bilayered molecular systems,"* May 20, 2013

JUNE 2013

George E. Arab (University of Rochester)
"Studies Toward the Synthesis of FK-506," June 5, 2012

Professor Ekaterina Pletneva (Dartmouth College)
"Becoming a peroxidase: conformational dynamics of a membrane-bound cytochrome c," June 17, 2013

Professor José Luis Mascareñas (Universidad de Santiago de Compostela, Spain, Center for Research in Biological Chemistry and Molecular Materials - CIQUS)
"Synthetic constructs for DNA and protein binding and sensing," June 24, 2013



Chemistry-Biology-Biophysics Interface Retreat

Professor Eric Kool (Stanford University)
"Designer DNA Bases as Probes for Biological Molecules and Processes," June 6, 2013

Dr. Payel Das (IBM)
"Exploring protein stability at multi-resolution," June 7, 2013

Sina Ghaemmaghami (University of Rochester)
"Conformational adaptation of synthetic prions," June 7, 2013

Nick Leioatts (University of Rochester Medical Center)
"Ligand mobility explains internal hydration and reconciles active rhodopsin structures," June 7, 2013

Chinmay Surve (University of Rochester Medical Center)
"G protein beta gamma is sufficient to induce directional chemotaxis," June 7, 2013

Josh Kolev (University of Rochester)
"Late-stage elaboration of the anticancer natural product parthenolide via chemoenzymatic synthesis," June 7, 2013

Dr. Hal Ebetino (Terpenoid Therapeutics)
"Advances in bisphosphonate drug development," June 7, 2013

Spring on campus

Distinguished & Special Lectures



¹ **Matthew C. Beard** Seymour Rothchild Lecture (October 2012)

² **Herbert Waldmann** Victor J. Chambers Memorial Lecture (February 2013)

³ **Darren J. Dixon** Andrew S. Kende Lecture (March 2013)

⁴ **David Milstein** Charles F. Hutchison Memorial Lecture (April 2013)

NEWS FROM THE ADMINISTRATIVE STAFF:

The staff enjoyed their annual summer outing at a Red Wings Baseball game this past July – and the team won! The weather was perfect - not raining or too hot. We enjoyed cheering the team on, especially **MARINA TOKINA**, editorial assistant to Oleg Prezhdo (currently editor for three journals). Thanks to Barbara Snaith for organizing this trip. The food, of course, was delicious!

KATE REINHARDT is finishing her first year in the chemistry department. Kate and Elly work together in prepping the undergrad labs as well as shipping and receiving for the department. Kate also TA's for the undergraduate labs, distributes the dry ice and gas cylinders, as well as inspects the research labs for safety compliance. She has just started this fall in the Simon School of Business Professional Masters in Business Administration Program. Besides taking classes part-time and working in the department, she teaches kickboxing classes for U of R Intramurals at the River Campus Gym and is involved in both a basketball and kickball league!

DEB CONTESTABLE is the Undergraduate Studies Program Coordinator and Course Administrator for the Department of Chemistry, having started in February 2012. Working with the undergraduate studies committee, Deb helps to ensure students are on track with their major/minor requirements and other coursework needs. She also works closely with the registrar's office and faculty regarding course scheduling and all other course related matters. Her responsibilities include coordinating the chemistry commencement ceremony, cluster retreats, as well as orientation & recruitment affairs. Now that she is CLASP certified, she will also be assisting faculty in pre-proposal grant preparation, working closely with Terri Clark. On a personal note, Deb and her husband have two boys. Her 11 year old is beginning middle school, while her older son is beginning to drive. Both boys play cello, are active in sports, and keep Deb and her husband very busy - in a good way!

TERRI CLARK, now completing her fifth year with the department, and nearly two years as the Development Administrator (which includes Alumni Relations), enjoys working with faculty on grants and awards within the department, as well as keeping up with alumni. This past

year she and her husband, Ben, welcomed new grandson Owen Danger Clark to the family – born to oldest son, Joe, and his wife, Kristy right before Christmas! This June, youngest son, Andrew, graduated from Eastern Oregon University, got married, honeymooned in Germany in July, then moved to Bellingham, Washington to start graduate school at Western Washington University. A busy year!



Donna and brother, Robert

DONNA J. DOLAN is a long time staff member in the Department of Chemistry. She is currently beginning her twenty-sixth year in chemistry, serving as departmental receptionist. 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 speakers program. Donna is also a proud owner of an XL883L Harley Davidson and enjoys riding with her brother, Robert West.

ROBIN COOLEY, our graduate studies coordinator, has now been with the department for nine years. She continues to coordinate 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 night of fun and games at the Strong

Museum of Play hosted by the current graduate students, followed by a full day of activities including tours, faculty talks and socializing. Each fall, Robin also organizes a week long orientation event for all incoming graduate students. This is a busy week designed to get all of the new graduate students informed and ready for the start of the new school year. For the 2013-2014 school year, we are welcoming twenty seven new graduate students to the department.

LYNDA MCGARRY (M.S. '85) is the administrative assistant to Professor Lewis Rothberg, the new chair of the Materials Science program, who takes the helm of the interdisciplinary program from outgoing chair Todd Krauss, Professor of Chemistry and Optics. Lynda coordinates graduate student admissions for the program, which will welcome three doctoral and eleven master's degree students this fall, for a total of 15 PhD and 23 MS degree students. Lynda'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. Lynda organized the successful "Nanosymposium 2013 –Novel Materials for Sustainable Catalysis" that was held on May 20, 2013, as well as the Materials Science Seminar Series held jointly with other departments throughout the year. In addition to her Materials Science program duties, Lynda works part-time as an editorial assistant in both the JACS and the JOC offices, and really appreciates all that she continues to learn about the journals from Valerie and Terrell. Lynda and her family like to watch lacrosse, snowmobile, and spend time at their cottage on Port Bay with family and friends and their schnoodle.

KENNETH SIMOLO (PH.D. '85) starts his twenty-sixth 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. While a graduate student here at the U of R, he earned his doctoral degree under the direction of George L. McLendon. Ken continues to work on updating the business accounting software for the Department to eventually become completely web based and keeps us on top of safety measures in the labs.

BARBARA SNAITH completed her second 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 coordinating paperwork as it relates to new faculty recruiting, attending monthly faculty meetings and preparing the discussion minutes. She also manages the immigration obligations needed for the Department's incoming postdoctoral research associates, many of whom are foreign nationals. In her spare time, Barb enjoys fundraising for causes about which she is passionate, such as the Lollypop Farm, as well as going to the GEVA theatre with her good friends. She is a very active member of her church, chairing fundraisers and women's events. She lives in Gates with her adorable white cat named Snowball!

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



Aaron Timothy York

graduate of Alfred University and has a Master's degree in education. She has clinical experience, having previously worked in several veterinary clinics prior to coming to the UR. On July 8th, Elly and husband, Brandon, celebrated their son Aaron Timothy's second birthday!

MARGUERITE WESTON, assistant to faculty, has been with the Department of Chemistry for eighteen years. She coordinates Chemistry's seminar program by scheduling rooms, contacting speakers to ensure their travel arrangements are in place, obtains their titles and abstracts, prepares 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 assists Professor Thomas Krugh with the many administrative details of Chemistry's National Science Foundation supported annual summer research program for undergraduates (REU). This includes assisting in the preparation of competitive renewal proposals for each three-year period and annual reports. Our most recent proposal of 2011 was approved by NSF for three-year funding. This

program attracts approximately 100 applications each year from undergraduates across the nation and the University of Rochester. Marguerite and husband, Art, are residents of Henrietta, NY, and enjoy dancing and gardening.

NEWS FROM 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. The business office staff consists of four members with valuable experience.



Chris & Oksana Kuitems

ANNA KUITEMS is responsible for reconciling grant ledgers, P-card management and graduate student payroll, and as backup for Randi Shaw. Anna celebrated her ten years of service with the university this year. Anna and her husband traveled to London this Fall to visit their daughter Megan. Their son, Chris, joined them from Kazakhstan. They later then traveled to Kazakhstan for their son Chris' wedding on June 29, 2013, to Oksana Kanalash. She is looking forward to having both of them back in the states in the near future.

RANDI SHAW, part-time chemistry accounting bookkeeper 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 nine 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 28 years now.

NEWS FROM THE EDITORIAL OFFICES

TERRELL SAMORISKI began her ninth year as editorial assistant for *The Journal of Organic Chemistry (JOC)* this August, 2013. She works closely with Professor Robert K. Boeckman, Jr., associate editor for *JOC* and continues to enjoy her work in scientific publishing. Her previous position as structure editor for the *Chemical Abstract Service* also involved the processing of scientific information. She enjoys working with part-time journal assistant **LYNDA MCGARRY (M.S. '85)** whose breadth of scientific knowledge is an incredible resource. The *JOC* publishes original contributions reporting novel, important findings of fundamental research in all branches of the theory and practice of organic chemistry. In 2012, the Rochester office handled about 300 manuscripts submitted to the Journal. As a direct result of the contributions of the *JOC* Editors and staff, the Thomson Reuters Impact Factor increased to 4.564 and again set a new standard.

The *Journal of Organic Chemistry* publishes shorter articles (Notes) and lengthy ones (Articles) along with synopses and brief communications for the American Chemical Society. In 2012 the Journal published two special issues to honor both Robert Ireland and Howard Zimmerman. The covers of the journal continue to be a highly desired forum for authors to showcase art relating to their manuscripts.

Seven of Diane Visiko's nine grandchildren



VALERIE FITZHUGH continues to enjoy working with Prof. William D. Jones as Editorial Assistant with the *Journal of the American Chemical Society (JACS)*, and expects that approximately 500 manuscripts will be assigned to this office in 2013. After 10 years with *JACS*, she still finds the fast pace of the journal office engaging and interesting, and enjoys working with part time assistant Editorial Assistant **LYNDA MCGARRY (M.S. '85)** who continues to be a valuable resource for *JACS* with her extensive knowledge of science. *JACS*, founded in 1879, is the flagship journal of the American Chemical Society and the world's preeminent journal in all of chemistry and interfacing areas of science. This periodical is devoted to the publication of fundamental research papers and publishes approximately 19,000 pages of articles, communications, and perspectives a year. Published weekly, *JACS* provides research essential to the field of chemistry. The most cited journal in chemistry, the *Journal of the American Chemical Society (JACS)* received 431,286 total citations and an increase in Impact Factor to 10.677, as reported in the 2012 Journal Citation Reports® (Thomson Reuters, 2013)

After twelve years, Editor-in-Chief, Richard Eisenberg, Tracy Harris Professor Emeritus, retired and the UR office of the journal, *Inorganic Chemistry*, closed its doors on December 31, 2012. **KIRSTIN CAMPBELL** left the office in the middle of December and **ARLENE BRISTOL** was scheduled to retire the end of February 2013. However, Arlene was diagnosed with acute myeloblastic leukemia in November and went on disability for six months. She returned to work on May 2nd and Arlene and Rich cleaned out the office during May. She formally retired from the University on June 1st after having worked over 55 years in Chemistry Departments at the UR, Michigan, and Princeton. The department celebrated her retirement with a special luncheon at Panzari's Restaurant in the Corn Hill district of Rochester.

SCIENTIFIC & TECHNICAL STAFF

TERRY (TED) O'CONNELL finished his thirtieth year with the chemistry department and still enjoys his position as director of technical operations. He is responsible for new equipment installations and any building renovations. **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 at the obgyn and anesthesiology departments. Prior to coming to Rochester, he worked as a research chemist at NYU, Nelson Institute of Environmental Medicine (90-95). He has peer reviewed research publications and patents both with the

University of Rochester and the New York University. This past spring he won the department Sandra Beach Award!



Eric & Jeanne Lobenstine

ERIC LOBENSTINE (PH.D. '81), manager for computers and network, is happy to report a year with no major problems, and some distinct successes. The new email/web server installed about 15 months ago is wonderfully easy to maintain. As a result, Eric has reduced his contract with University IT for system administration backup, saving the department a bit of money while keeping just enough time to cover an emergency while he is on vacation. Also, availability of funds from the Dean's Office allowed upgrading the network for all faculty and staff offices to gigabit speeds, ten times faster than our old network. This was a major project - two installers for almost 3 weeks, 4 miles of cable, \$6000 in new network hardware - and came off without a hitch. He admits that this will mostly be useful for those who participate in video conferencing, but the installation of all new cables and switches means that he'll have fewer worries as the rest of our network infrastructure continues to age. Eric continues to represent Chemistry's interests on numerous IT committees within the University, and finds it interesting to see how IT challenges shift with time, even if they do not directly affect our operations. A recent "spear-phishing" attack on major universities throughout the country snared a few victims at the University and, as a result, compromised some accounts within the HRMS system. Remember - NEVER click on a web-link in a message that you were not expecting to receive! The black hats are getting very good at making emails look very realistic!

On the home front, older son Brian finished his trainee year with Parker, and accepted a Customer Service Manager posi-

tion in the Boston area, which he is enjoying greatly. How someone goes from being a trainee to managing a group of 15 employees baffles me, but he seems to relish the challenge, mostly. He has to supervise his first termination soon, and is not looking forward to it. Finishing his Take 5 year, Ethan graduated magna cum laude from the UR in May and has returned home to puzzle out his next steps. He seems pretty clear that he wants to direct a high-school or college choir, eventually, and is feeling his way along the start of that path. Jeanne and Eric agree that, while it is sad to realize that the nest will be truly empty soon, it is wonderful to see our sons finding their way in the world.

RAY TENG (B.S. '83, M.S. '87, M.B.A. '01) has been with the University since 1987 and joined chemistry in 2004 as research/facility coordinator. Ray brings many years of experience to the department, having previously worked in the Department of Physics and Astronomy, the Nuclear Structure Research Laboratory, and the Department of Earth and Environmental Sciences as senior technical associate. Ray continues to enjoy the daily interactions with faculty and students in addressing research and facilities issues. Soccer continues to play a big part in Ray's spare time watching his daughter play D3 soccer.

This past year saw an increased demand for X-ray diffraction and elemental analysis experiments. As manager of the facilities, **BILL BRENNESEL** kept very busy juxtaposing the evaluation of research samples with instructional duties. In the X-ray facility Bill analyzes single crystalline samples (like sugar or salt crystals, but of new materials designed by the synthetic chemists) to provide researchers with a confirmation of the newly proposed materials, as well as the positions of the atoms in three-dimensional space throughout the

Carlsen Library stacks



crystal. This characterization technique is very useful for the publication of new molecules. This year Bill taught the annual graduate course in X-ray diffraction (CHM/MSC 416) from which a dozen newly trained users of the facility were produced. Students in the course, who come from a variety of backgrounds including optics, engineering, and chemistry, learned the basic theory of X-ray diffraction and its application via real experiments and the modeling and reporting of the collected data. Undergraduate students in the advanced laboratory techniques course (CHM 234) also spent time in the X-ray facility. They practiced how to select and mount crystalline samples, from which they collected unit cell data (an "X-ray fingerprint") to be checked against a database of known materials. This past year Bill has also continued collaborating with professors from local colleges, including Professor Bradley Kraft from St. John Fisher College and Professor Steven Tajc from Nazareth College. The elemental analysis facility (which determines the percentages of carbon, hydrogen, and nitrogen in a bulk research sample) has nearly doubled its number of analyzed samples from the previous year with the addition of submissions from new research groups and an increase in submissions from current ones. More and more, students and faculty are appreciating the convenience of having a facility of this nature in the chemistry department. Over the past year Bill has analyzed over 500 solid and liquid samples, many of which are air-sensitive and have to be handled in a glove-box filled with the "inert" gas argon; such samples react with the oxygen and/or water vapor in the air we breathe.

SUE CARDINAL, chemistry librarian from the Carlson Library, reports that the library has subscribed to our first "app" called BrowZine which delivers thousands of academic journals through a free iPad app. We've also added electronic access to the ACS Symposium Series. A new Data Librarian, **KATHLEEN FEAR** with a BS Physics from Yale, MS in Information and recent PhD in Information



Sue Cardinal

from University of Michigan, has started and she will help researchers manage, secure and share their data and write data management plans. The second floor of Carlson has been renovated, adding colorful seating, and more collaborative space amongst fresh carpet and paint. We continue to hold "study break" parties during finals week to boost the student's efforts with comradery, sugar and caffeine.

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 NMR Spectrometer
- ~ Brüker 500 MHz NMR Spectrometer
- ~ Two Brüker 400 MHz NMR Spectrometers
- ~ Brüker 300 MHz NMR Spectrometer

Mass Spectrometers:

- ~ Brüker 9.4 Fourier Transform Mass Spectrometer (FTMS)
- ~ Thermo LTQ Velos Ion Trap LC/MS
- ~ Brüker Autoflex III SmartbeamMALDI-TOF
- ~ Shimadzu GC/MS, with AOC-20i autosampler & dual columns, + & - CI
- ~ Shimadzu GC/MS, with Direct Inject Probe, + & - CI
- ~ Shimadzu LC/MS, with APCI & Electrospray ionization sources

Laser Systems:

- ~ Transient absorption systems based on a picosecond Nd:YAG laser and a nanosecond excimer-pumped dye laser
- ~ Picosecond time-correlated single photon counting fluorescence system based on a Nd:YLF-pumped cavity-dumped dye laser
- ~ Nd:YAG/dye laser system
- ~ Associated optical instruments:
 - monochromators and spectrographs
 - fast multichannel plate photo-detectors
 - state-of-the-art, highly sensitive array detectors (CCDs and photodiode arrays)

Other Instruments Include:

- ~ Brüker EMX-Plus EPR spectrometer with 4 K temperature capability
- ~ CEM Explorer Microwave Synthesizer
- ~ ThalesNano H-Cube continuous-flow hydrogenation reactor
- ~ Perkin Elmer 2400 CHN/S Analyzer with VAC Atmospheres (Argon) glove box
- ~ REACT IR; infrared with probes for monitoring and recording spectra over time
- ~ Brüker X-Ray Diffractometer, with Apex II CCD area detector
- ~ Perkin Elmer Lambda 950 UV/VIS Spectrometer
- ~ Perkin Elmer Lambda 35 UV/VIS Spectrometer with Peltier temperature control unit
- ~ Shimadzu 6300 Atomic Absorption Spectrometer
- ~ Five Shimadzu FTIR spectrometers
- ~ Single molecule time-resolved fluorescence confocal microscope
- ~ Thermogravimetric analysis and Differential Scanning Calorimetry for polymer characterization
- ~ Digital Instruments Nanoscope Ila Atomic Force Microscope
- ~ Ellipsometer
- ~ Spectrofluorometer from Roper Scientific, infrared and visible
- ~ Phosphoimager

Organic Chemistry students in lab (J. Adam Fenster)



Departmental Funds

You may also donate online at <http://www.chem.rochester.edu/alumni/giving.php>

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 the purchase of undergraduate laboratory equipment, assisting graduate students with travel expenses to scientific conferences, and supporting Chemistry's outside speakers program.

Distinguished Lectureship Funds

These lectureship funds are designed to bring scholars distinguished in their field to the department for a series of lectures and to meet with faculty and students.

Victor J. Chambers Memorial Lectureship honors an early chairman of the Department of Chemistry.

Hutchison Memorial Lectureship honors Charles F. Hutchison, Class of 1897, who donated funds for Hutchison Hall.

W. Albert Noyes, Jr. Memorial Lectureship honors Professor Noyes, former chairman of the department, dean of the Graduate School and dean of the College of Arts and Science.

Richard Eisenberg Chemistry Endowment

A new fund to honor the distinguished career contributions of Richard S. Eisenberg, the Tracy H. Harris Professor of Chemistry.

The Chair of Synthetic Organic Chemistry, Honoring Andrew S. Kende

Established in 2006 to honor the distinguished career contributions of C. F. Houghton Professor Emeritus Andrew S. Kende.

Magomedov-Shcherbinina Memorial Fund

Establishes an annual research prize in memory of the Magomedov Family, who were tragically killed in 2006.

Jack A. Kampmeier Fund for Peer-Led Workshop Education in Chemistry

Established in 2005 to honor Professor Kampmeier's 45th year of teaching, this fund supports initiatives that strengthen the Peer-Led Workshop program.

Marshall D. Gates, Jr. Chair in Chemistry Fund

Established in 2002 to honor Marshall D. Gates, this fund helps finance research for the chair holder.

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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 online at http://www.chem.rochester.edu/alumni/update_contact.php

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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