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Greetings to all Department of Chemistry Alumni! We enjoyed a busy and productive 2010-2011 year in the department and at the University. As I enter my ninth 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 some 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 payout. The University Endowment has largely recovered from the events of 2008, but the College's (including the College of Arts, Sciences, and Engineering) draw on their portion of the 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 for the undergraduate program is on track. Since the chemistry department anticipates that a proportionate number of incoming freshmen will participate in the chemistry curriculum and we have had one retirement, we have been able to add two tenure-track faculty (one senior and one junior) and one instructor in 2010-2011. Furthermore, despite an ailing economy, the department has increased in sponsored research to \$4.9M in 2010 and UR chemistry alumni have continued their strong, generous support of the

departmental funds.

As a central science, chemistry has an essential part to play in the nation's research enterprise. 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, PRF, NSF, and the Sloan Foundation 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 for 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. NIH and NSF funding levels 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.

New research initiatives, such as those in systems biology, nanotechnology, renewable energy (particularly fuel cell and hydrogen production), and identification of gene function, are clearly areas of critical importance to the nation. Such research areas, in which the University and our department are well positioned to participate, coupled with the expected growth in the student body and a maturing demographic among our senior faculty, will require the continued hiring of new faculty. The growth target, although now some years in the future, is 24-26 full-time tenured or tenure track faculty. Such growth is critical to allow the department to compete effectively against our peer chemistry departments, almost all of whom are larger than Rochester, for the best faculty and graduate students.

Fortunately, as mentioned above, chemistry was selected as one of the departments permitted to make a tenure-track faculty hire this year, in one of the tightest budgetary years of any, save next year (2012-2013). We were exceedingly pleased to have attracted a superb young inorganic chemist Michael Neidig as assistant professor of chemistry. Mike received his Ph.D. training under Ed Solomon at Stanford, and spent a year in industry at Dow Chemical. At that point, he decided to pursue an academic appointment and moved to a postdoctoral position at Los Alamos National Laboratory. Mike will pursue a research program spanning mechanistic inorganic and organometallic chemistry using spectroscopic methods, particularly cryogenic magnetic CD and Mossbauer spectroscopy, as platforms for these studies. His research program has an unusual level of synergism with Pat Holland, Bill Jones, and other chemistry faculty which made him a perfect fit for Rochester. We are excited to have him. We have also hired a recent alumnus **BENJAMIN HAFEN-STEINER (B.A. '03)**, who received his Ph.D. at Scripps with Phil

Baran and a postdoctoral stint with Larry Overman at Irvine, as an instructor who will focus on instruction of our freshman and sophomore level lectures and laboratories. Ben's background and skill in synthetic organic chemistry will also benefit the research programs of several organic chemistry faculty.

Chemistry faculty received several notable awards this year, the details of which you will read in this newsletter. Most notably, Esther M. Conwell received a National Medal of Science at a White House ceremony. This was the first in the history of the University of Rochester. Rich Eisenberg was inducted into the National Academy of Sciences. David McCamant was named a recipient of a prestigious Sloan Foundation Research Fellowship. 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 the 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 an unprecedented seven NSF Graduate Research Fellowship Awards and Honorable Mentions. Efforts to remain on the cutting-edge of research and education are ongoing, as you will read about in the rest of the newsletter.

We were saddened this year by the loss of Professor Emeritus Jack A. Kampmeier who passed away in March. Throughout his long career here at the University of Rochester, beginning in 1960, Jack dedicated himself to the education of all students; to use his phrase, "from freshmen to postdoc". He inspired faculty here and elsewhere to raise their teaching to new levels of excellence, having helped pioneer the "Peer-Led" Team Learning workshop model. He was still very active on campus even though he retired in 2005. Jack was an esteemed colleague, an excellent communicator, a visionary and passionate leader, an untiring advocate for students, and an exemplary citizen of the University community. His passing leaves a hole in our chemistry "family". We will all miss him.

In January 2009, chemistry launched its newly redesigned website. We are proud to showcase our department with this informational internet presence which is now more accessible and utilizes more links, cross references, quick facts, and substantially more graphic detail. The contemporary site is not only more attractive and standards-compliant, but has greater functionality and security built into its administrative system. Alumni are invited to visit us at www.chem.rochester.edu. The newsletter is also available online and we will continue to develop the overall website.

We were pleased to have been able to make some significant improvements to our departmental infrastructure this year with the completion of construction of a new undergraduate organic laboratory in Hutchison Hall. This laboratory will serve as a model both for future renovations of our remaining organic laboratories and a basis for planning renovations of our freshman laboratories, but also for fund-raising efforts for these renovations as part of the University's major gift campaign set to begin in October. Through such generous gifts of our alumni and other university and unre-

stricted funds, we will continue the staged renovation of chemistry's research and teaching laboratories over the next several years.

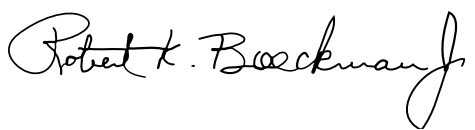
For many years we have aspired to grow our graduate program. I am happy to report that again this year chemistry has experienced sustainable growth in our graduate program with the matriculation of 17 new first year graduate students bring our departmental graduate student population to about 120 and our total researchers to over 150.

Finally, let me close by thanking all of you for your continuing support of the department over the year. We are fortunate to have the strong support of the College in all our efforts, however, the support and advice of our alumni is an invaluable resource. We are happy to receive news and 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. Please remember to update your contact information (you may do so now online) as you move from place to place, and stay in touch with your alma mater!

One of the defining characteristics of the Department of Chemistry at the University of Rochester is our warm relationship with chemistry alumni and our collegial atmosphere. Over the years, we have endeavored to establish and nurture the sense of community for our alumni. We encourage you to take this opportunity to acquaint yourself with current members of the department and reconnect with old classmates, through the newsletter, through attending events, and through our website. We greatly appreciate your communication and feedback and moreover, want our current students to appreciate the legacy of our extended "Chemistry Family" through a bond with their predecessors. We invite you to visit Rochester, attend Meliora Weekend events, including the infamous Gates Happy Hour, and drop by our next ACS Alumni Social Hour to be held at the Philadelphia ACS National Meeting in August 2012.

Meliora and best wishes to all for a successful and happy year in 2011-2012.

Sincerely,



Bob Boeckman, Jr.

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Includes donations received between July 2010 and June 2011.

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Noal Cohen (B.S. '59)
 Richard P. English (B.S. '65)
 John Figueras (B.S. '49)
 Thomas J. Perun (Ph.D. '63)
 Margaret May-Som (M.S. '74, Ph.D. '76) and
 Wu-Yong Wu (Ph.D. '74)

CORPORATE CONTRIBUTIONS...

Abbott Fund Matching Grant Program
 Astrazeneca
 Bristol-Myers Squibb Co.
 Chevron Corporation
 E.I. Du Pont De Nemours & Company
 Eli Lilly and Company Foundation
 Exxon Mobil Corporation
 Johnson & Johnson
 Jones Day
 KBN Optics LLC
 Meet the Composer
 Merk & Co., Inc.
 Microsoft Corporation
 Neenah Paper, Inc.
 Novartis Pharma AG
 Shell Oil Company Foundation
 Texas Instruments
 Zeon Chemicals USA, Inc.

In recognition of his continuing commitment and service to the university, **LOU LANGE (B.A. '70)**

received the 2010 Distinguished Alumnus Award, School of Arts & Sciences.

He joined the University Board of Trustees in 1997 and has actively served as chair or member of several board committees. For five years as the Chair of the Health Affairs Committee, Lange was part of the leadership team for strategic re-energization of the medical center, to construct two research buildings and recruit over 100 faculty members. He is also a charter member of the George Eastman Circle, the University's leadership annual giving society. Lange is widely recognized as an expert in the field of molecular cardiology with his 22 years of experience in academic medicine. Lange is a general partner at Asset Management, an investment firm in Palo Alto, CA. He founded CV Therapeutics Inc. in 1992 and is the former chairman, chief executive officer and chief scientific officer.



In July, **PETER R. BERNSTEIN (B.S. '73)** retired from AstraZeneca Pharmaceuticals after thirty-one years of service. This was earlier than he had planned and was in conjunction with the closure of the research site at which he had worked. He looks forward to having more time for family, friends and hobbies.

ELLIS GLAZIER (PH.D. '57) has been living in La Paz, Mexico for 22 years. The first two were spent unwinding from the fast-paced life in California. Baja, California is a different world. For almost 20 years now he has been working as an author's editor, editing papers written in English by mostly Mexican scientists, with the odd sprinkling of Russian, Israeli, and other Spanish-speaking workers from Central and South America, Cuba, and Spain. Most of his work was in marine biology and terrestrial biology, but for a number of years now he has been working on papers about human medicine and gene splicing. All of this has been quite an education for an organic chemist. Glazier would suggest this kind of work to anyone who wants to keep one's mind active and stay alive past the three score and ten that used to

be the norm. It is also something that one can do well in, though it is necessary to get some background from experienced editors and also to stay up to date on the ever changing world of scientific style and format. Fortunately, he worked for Marshall D. Gates and had a real editor as his guide.

GORDON A. NICHOLLS (POSTDOC '52) of Auckland, New Zealand recounted that he was the first person to go from New Zealand to the United States as the holder of a U.S.P.H.S. post doctoral fellowship. He has retired and is focusing on writing about his travels and life experiences. The world was a different place in the 50's. He remembers Marshall D. Gates fondly.

SAM THOMAS (B.S. '00) just completed his 2nd year as assistant professor of chemistry at Tufts University, where he joined as a member of the faculty after completing his Ph.D. with Tim Swager at MIT in 2006 and an American Cancer



Society Postdoctoral Fellowship with George Whitesides at Harvard University. Since forming at Tufts, the Thomas Lab, which numbers seven people, has reported a new class of photo-responsive materials that switch electrostatic properties upon irradiation, as well as new fluorescent polymers that sense singlet oxygen. Sam also received a DARPA Young Faculty Award and a Synthesis-Synlett Journal Award.

ERWIN KLINGSBERG (PH.D. '44) is a member of the NJ Hall of Fame. His age discrimination suit against American Cyanamid was the subject of a symposium held at the 1994 ACS meeting in Washington. The knowledge of the U.S. legal system, gained from his experience, is proving valuable in current litigation that is reshaping landlord-tenant relations in Washington, DC, where he lives with his wife of 66 years, the former Anna Strauss, herself a chemist holding degrees from the ETH in Zurich and Columbia University. Their virologist daughter, Dr. Dinah Bodkin, was recently awarded a substantial sum in settlement of a lawsuit arising out of her dismissal, without just cause, by Harvard University.

MARCY BALUNAS (B.A. '95)

is currently an assistant professor in medicinal chemistry at the University of Connecticut. After earning a double B.A. in chemistry and biology at the UR, Marcy went on for a M.S. in plant ecology at SUNY College of Environmental Science and Forestry and a Ph.D. in pharmacognosy at the University of Illinois at Chicago. Marcy just completed a postdoctoral fellowship at the Scripps Institution of Oceanography in conjunction with the Smithsonian Tropical Research Institute. Marcy's lab focuses on selectivity-based anti-parasitic and anti-cancer drug discovery from marine microorganisms with a focus on psychrophilic bacteria, including synthetic modifications of natural product isolates, as well as elicitation of silent biosynthetic pathways in cold-obligate bacteria.



THOMAS NASHERI (B.A. '98, TAKE 5 '99) is currently completing his last year of residency in internal medicine at University Hospitals Richmond Medical Center in Cleveland, Ohio. Recently he won first place, Resident Poster Contest, at the 2010 American College of Osteopathic internists (ACOI) Annual Convention and Scientific Sessions in San Francisco, California. His poster was titled "Hyperammonemic Encephalopathy in Multiple Myeloma." He will be looking for a career in hospitalist medicine in the Cleveland area after residency.

DEVIN RUIZ (B.A. '10) started medical school at Thomas Jefferson University in August. As an undergraduate in the chemistry department, he led workshops. He believes that the experiences he gained throughout the time as a workshop leader helped him get into his top choice medical school and will continue to be helpful in the years to come.



MARTIN ZANNI (B.A. '94, B.S. '94), professor of chemistry at the University of Wisconsin, Madison, is the winner of the 2011 Raymond and Beverly Sackler Prize in the physical sciences. Marty was selected for his contribution to the ultrafast spectroscopy field. Additional awards in 2011 include the H. I. Romnes

Faculty Fellowship from the UWM and the NAS Award for Initiatives in Research. As a note, **SHAUL MUKAMEL**, for-

mer chemistry department professor spoke at the 2011 Sackler Symposium.

KYLE BULICZ (B.S. '09) began a chemistry doctorate program at the University of Utah last fall. He was admitted to the program with a graduate teaching assistantship, as well as a full academic scholarship. In addition to a Bachelor of Science degree in chemistry at Rochester, he also received a minor in biology. During his senior year, he conducted research with Professor Turner in the field of biophysics, studying the presence of imino proton energy exchange in base pairs flanking single nucleotide bulges in RNA duplexes. He was the president of the undergraduate chemistry council as a senior and won the prestigious Carl A. Whiteman Excellence in Undergraduate Teaching Award. He was a TA for three labs: General Chemistry 132, Organic Chemistry 207 and Honors Organic Chemistry 210.

STEPHANIE CHIU (B.A. '07) has begun her first year as an intern as part of the St. Anthony Family Medicine Residency program. After graduating from the University of Rochester with a double degree in chemistry and molecular genetics, Stephanie attended the University of Cincinnati for medical school. She is exploring careers in hospital medicine and geriatrics.



Breanne Holmes

BREANNE HOLMES (B.S. '08) has enrolled in the graduate chemistry program at the University of Massachusetts Amherst. Her senior thesis work was under Professor Kara Bren, studying and making mutations of *H. thermophilus* cytochrome *c*. She also had the pleasure of working with Professor Bill Jones.

IN MEMORIAM

As the previous newsletter went to press, we were saddened by the news that Professor Jacob Bigeleisen, former chair of the chemistry department from 1970-1975, passed away at age 91.

In honor of Jacob Bigeleisen's life and work, a Symposium & Memorial on Isotope Chemistry was held on April 29, 2011 in Maryland. Faculty members Rich Eisenberg and Bill Saunders attended the event. Among his major accomplishments as chair included



the ranking by the American Council of Education of the chemistry department as one of the strongest in the nation. In 1972, the department moved from Lattimore Hall to its current home in Hutchison Hall. The series of Departmental Visiting Distinguished Lectures, including the Dreyfus lecture series and Hutchison lecture series, began during his time as chair.

Bill Saunders (center) attends the Bigeleisen Symposium



ROBERT LUIS AUTREY, scientist and noted collector of early acoustical recordings, died Sept. 4, 2011, in Portland, at age 79. Although he had been in declining health for more than a decade, he was energized by his enthusiasm for musical performances, intellectual interests and reverence for nature. Robert grew up in Galveston and Houston, Texas, where he attended the Kinkaid School. He began his undergraduate work at Rice University, and obtained his bachelor's degree from Portland's Reed College in 1953. He completed his Ph.D. in organic chemistry at Harvard in 1957, and a postdoctoral fellowship at Imperial College, London, in 1958-59. Beginning in 1960 he taught chemistry at the University of Rochester for five years, and served as the assistant editor for the *Journal of the American Chemical Society*. He returned to Harvard for two years, and then to Oregon permanently, as a founding faculty member at the Oregon Graduate Center, subsequently known as the Oregon Graduate Institute. He left the Oregon Graduate Center to





Susan B. Anthony Hall, early 50's

become a partner in a scientific publishing venture, recognized for pioneering works on ecology. For several years he served as director of Research and Development at NERCO, then a subsidiary of Pacific Power.

HILLARD E. FIRSCHEIN (PH.D. '58), a biochemist from Sarasota, Florida, died in December of 2010. He received his undergraduate degree at Ohio State University and his masters at University of Wisconsin, Madison before receiving his Ph.D. in biochemistry at the University of Rochester. A veteran of the Korean War, he served in the Army at Oak Ridge National Laboratory located in Tennessee. In 1972, he became a director of clinical testing at Ciba-Geigy in Summit in New Jersey, which focused on the anti-inflammatory drug Voltaren. After 21 years with the company, he retired. He was an emeritus member of ACS.

MARY E. SCHOTLAND CASTELLION (B.S. '55) passed away on September of 2010 after battling Alzheimer's disease. Castellion developed her passion for science and writing at the University of Rochester and after graduating, went on to work as an editorial assistant at the *Journal of American Chemical Society* for a year. She coauthored the textbook "Fundamentals of General, Organic, and Biological Chemistry", as well as a number of other science textbooks. She was a member of the National Association of Science Writers (NASW) and ACS, serving in leadership roles in both local and national chapters. She appreciated music and art and played clarinet for both the Darien Band and the Norwalk Symphony, where she also served as President of the Board of Directors for many years.

The Department of Chemistry also mourns the passing of:

- ☞ Wilfred W. Bowman (Ph.D. '68)
- ☞ George H. Brice (B.S. '50)
- ☞ Mary E. Castellion (B.S. '55)
- ☞ Wayne E. Feely (Ph.D. '57)
- ☞ John H. Hageman (B.A. '57)
- ☞ Robert E. Heeks (B.A. '52, M.S. '54, Ph.D. '57)
- ☞ Phillip Hoffman (Ph.D. '54)
- ☞ Edward H. House (Ph.D. '60)
- ☞ Kenneth O. Kutschke (Ph.D. '51)
- ☞ William E. Lovett (Ph.D. '56)
- ☞ Gerold A. Mancini (B.A. '51)
- ☞ Frances Z. Mayberry (B.A. '61)
- ☞ John F. Paulson (Ph.D. '58)
- ☞ Eugene J. Sehm (Ph.D. '58)
- ☞ Noel H. Turner (Ph.D. '68)
- ☞ Marshall E. Tyler (B.S. '50)
- ☞ William G. Webb (Ph.D. '54)
- ☞ John Williams (B.S. '49)

Interfaith Chapel



Esther M. Conwell receives National Medal of Science



Esther M. Conwell, professor of chemistry and physics at the University of Rochester, received the National Medal of Science from President Barack Obama during a White House ceremony on November 17th.

The National Medal of Science was established by Congress in 1959 and is awarded by the president to recognize “outstanding contributions to knowledge” in the sciences. A committee of 12 scientists and engineers, appointed by the president, nominates individuals for the National Medal of Science. The final decisions are made by the president. The Award is presented at the White House. Conwell’s honor represents the first National Medal of Science award for a University of Rochester faculty member.

“It’s no exaggeration to say that the scientists and innovators in this room have saved lives, improved our health and well-being, helped unleash whole new industries and millions of jobs, and transformed the way we work and learn and communicate,” President Obama said.

Conwell earned her master’s degree in physics at the University of Rochester in 1945 and her doctorate at the University of Chicago where she was an assistant to Nobel Prize winner Enrico Fermi. She did her doctoral work with another Nobelist, Subramanyan Yan Chandrasekhar. From 1946 to 1951, she taught at Brooklyn College, her undergraduate alma mater. She also spent a year as a visiting professor at the graduate school of the Sorbonne, L’École Normale Supérieure, University of Paris in 1962, and a semester at MIT in 1972 as the Abby Rockefeller Mauzé



Esther with family members, Lewis Rothberg, Shelby Nelson, Charles, and Vivian

highest honors a scientist or engineer can receive. Conwell is the only member of the University of Rochester to hold such a distinction. She also received an Honorary Doctorate of Science from the UR in May.

“Esther is one of the preeminent female scientists of her generation,” says Robert K. Boeckman, Jr., chair of the Department of Chemistry. “She has served as a mentor to countless female scientists and engineers over the years, and has worked tirelessly for the cause of equality for women in science and engineering. After a superlative career that now spans more than half a century, she is still actively serving as an ideal role model to young female scientists and engineers. She still works with students on a daily basis, even at 89.” Bob continued, “When she learned of the award, she was concerned that the activities might delay submission of her next journal article. When the UR press group sought to meet with her, she scheduled them around her student meetings. For the actual UR press announcement, she was glad it came after a student’s poster session she was attending. For Esther, it is always about the science.”

professor. From 1973-2000, she was a senior scientist in the Xerox Research Laboratories. Professor Conwell was married to the novelist Abraham Rothberg, now deceased, and is mother of fellow scientist Dr. Lewis J. Rothberg, professor of chemistry, physics and chemical engineering at the University of Rochester.

Conwell earned a Ph.D. in atomic physics at a time when few women were entering science and is considered a pioneer in creating opportunities for women in science classrooms and professional laboratories. Her innovative semiconductor research earned her a place as one of Discover magazine’s 50 Most Important Women of Science in 2002. Even half a century later, Conwell’s scientific breakthrough work on semiconductors is still important to the understanding of electron transport today.

Professor Conwell helped launch the computer revolution by explaining the effect of impurities and of high electric fields on electron travel through semiconductors. Her research earned her membership in the National Academy of Sciences, the American Academy of Arts and Sciences, and the National Academy of Engineering, among the

Esther at IEEE meeting, circa 1980



A Celebration in Honor of Richard Eisenberg

An event to recognize the many accomplishments in research, teaching, and mentoring of our colleague and friend, Rich Eisenberg was held May 20-21, 2011.

Over a hundred former students came together the weekend of May 20th and 21st for “A Celebration in Honor of Richard Eisenberg”. The “Richfest” weekend kicked off with a reception at the Eisenbergs on Friday night. During a time of constant rain in the Rochester area, the day of the reception the sky cleared up long enough to put up a tent and have a great party. The good weather continued through Saturday night of the weekend. Among the attendees were five people from the 60’s when Rich taught at Brown in Providence, RI. Many of the others had not seen each other in many years, coming from as far as Italy and England. For some of the more recent graduates, the event served as a mini reunion and allowed them to meet more of their fellow graduates.

The Symposium was an all day event in Goergen Auditorium. Harry Gray, Rich’s Ph.D. advisor, unofficially emceed the event with many ad libs throughout the day, bringing tons of laughter as he spared no one from his good humor. Speakers included Dan Nocera, Cort Pierpont, **GEORGE STANLEY (B.S. ’75)**, **SIMON DUCKETT (POSTDOC ’93)**, **DON BERRY (POSTDOC ’85)**, **ZACH TONZETICH (B.S. ’02)**, Harry Gray, **BILL CONNICK (POSTDOC ’98)**, Jim Ibers, **CLIFF KUBIAK (M.S. ’77, PH.D. ’80)**, and **GORDIE MILLER (B.S. ’82)**. Several speakers took turns at a bit of humor involving Rich over the years. All made mention of



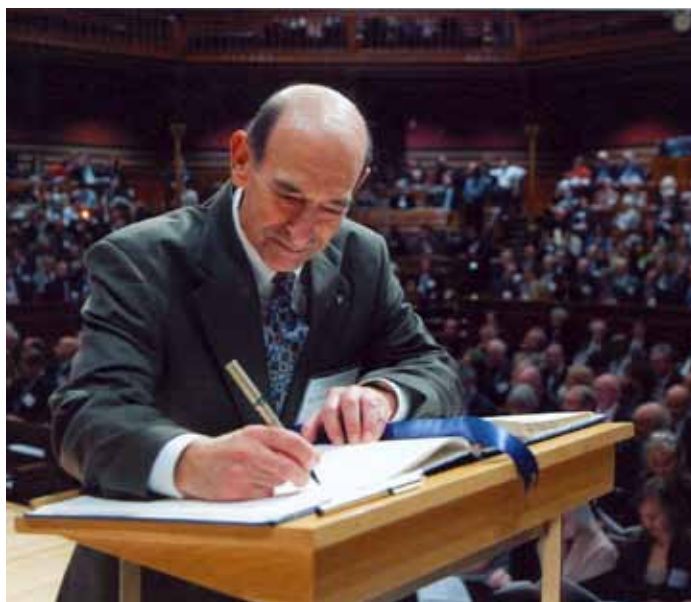
Symposium in Goergen Hall

Pingwu Du, wife Jing-Xue and son Alexander



the effect he had on them and his passion for chemistry. Several previously well kept secrets were also shared and the group roared almost continuously. In addition to the official symposium flyer, which was sent out to everyone before the event, an “ad libbed unofficial flyer” circulated during the day and can be found on the chemistry department website.

The Gala Dinner on Saturday evening began with cocktails in the Flaum Atrium at the UR Med Center. Rich also prepared a slide show of pictures for the group to enjoy. There were 120 attendees for dinner and the group picture is shown at right. Bill Jones and Jim Farrar organized the after dinner program and made it known that the person who really needed to be acknowledged was Marcia. Bob Witmer, John Sofranko, George Stanley and Cliff



Rich signing the National Academy of Sciences register



Gala Dinner in Flaum Atrium

Kubiak spoke from the heart about their time with Rich, the impact he had on their life and their thankfulness. After we thought we had heard it all, Harry Gray proceeded to tell even more stories about Rich. He brought Rich up to demonstrate “The Look” as the crowd burst into laughter. Rich gave a heartfelt talk to end the evening, talking about his life in chemistry, the relationships he had made and the things he had learned. Rich and Marcia left the next day for Prague for a continued whirlwind of travel. The year 2011 was a significant one for Rich as he was inducted into the National Academy of Sciences and we wish him the best in the next phase of his life!

Bob Witmer and Marcia



Gala Dinner Attendees



Department Mourns the Loss of Jack Kampmeier

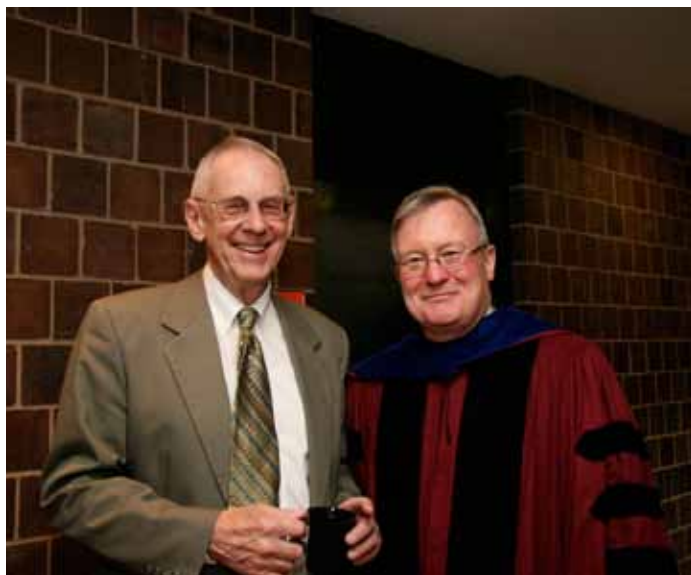


The department mourns the loss of Jack A. Kampmeier who passed away on March 26th. Jack accepted a faculty appointment in chemistry at the University of Rochester in 1960, after having received his A.B. (cum laude) at Amherst College in 1957 and his Ph.D. from the University of Illinois. He established a program of teaching and research in organic chemistry with an emphasis on organic reaction mechanisms

and free radical chemistry. His research group did seminal work on the structure and stereochemistry of vinyl radicals, and developed a powerful mechanistic tool for elucidating the mechanism of radical substitutions at nonsterogenic atoms. Nearly a decade later, Jack's research group turned their attention to organometallic reaction mechanisms. The Kampmeier group performed the key experiments to understand the decarbonylations of aldehydes and acid chlorides by rhodium(I). Their experiments ultimately led to a complete reinterpretation of the reaction mechanism and new, general insights into organometallic reaction pathways.

As an educator, Jack was a leader on the Rochester campus throughout his career. In the late 1960's, Jack initiated a complete revamping of the undergraduate chemistry curriculum. This led to new laboratory courses in organic chemistry and physical chemistry that emphasized the use of modern instrumentation and techniques. In addition, Jack invented, developed, and taught a new capstone course (CHM 234) that integrated

Jack and Jim Farrar at Commencement



previous laboratory work and prepared students for independent research. Jack was awarded the Edward Peck Curtis Teaching Award in 1974 for these curricular initiatives.

After having returned to the chemistry department from the Dean's office in 1991, Jack played a lead role in writing a successful proposal to the Hughes Foundation which led to the development of new courses in both the chemistry department and the biology department for students majoring in the sciences. Shortly thereafter, Jack began work on a pioneering educational initiative to develop and implement the Peer Led Teaming Learning model in his large, first semester organic chemistry course (CHM 203). In this model, students meet in small Workshop groups each week under the guidance of a peer leader to work on specially designed problems that actively engage them in discussion and debate. Experience has shown that students thrive in Workshop because it provides them a supportive place to express their ideas, test their opinions, and construct their own views on the subject material. Their engagement with the course material results in better student performance and greater satisfaction with the course.



Jack was an evangelist for the Workshop model for over fifteen years, both here at Rochester and across the country. At Rochester, the Workshop model has spread to more than fifteen courses in seven departments – far more than any other university or college in the country. It is rapidly becoming a signature of an undergraduate education at Rochester. The model is now being used at more than 100 colleges and universities that organize ca. 2,000 peers to lead Workshops for at least 20,000 students per year. Jack's success at developing and disseminating the Workshop model was recognized by the University with a Goergen Award for Artistry and Achievement in Undergraduate Teaching (1999) and by the Chemical Manufacturers Association's Catalyst Award for Excellence in Science Teaching (1999). In 2008, three years into his retirement, Jack shared the American Chemical Society's Jack Flack Norris Award for Outstanding Achievement in the Teaching of Chemistry with Professors David Gosser (CUNY, City College) and Prahtiba Varma-Nelson (Indiana University-Purdue University, Indianapolis).

Jack chaired the chemistry department from 1975 to 1979 and served as Dean of the College of Arts and Sciences from 1988



Jack and Anne Kampmeier



Joe Dinnocenzo speaking at the Memorial Service

to 1991. As chairman of the chemistry department from 1975-79, he successfully identified and recruited outstanding young faculty to the department, and organized the financing and acquisition of the first high field NMR spectrometer on campus. He encouraged and expanded the postdoctoral program in chemistry and established the idea of teaching postdoctorals. As chairman, he was also a member of the leadership committee that established the Rochester Plan.

In 1982, Jack accepted a position as the Associate Dean for Graduate Studies. He encouraged the aggressive recruiting of students in all graduate programs, in part supported by special graduate fellowships. From the period of the early 80's to the late 80's, the number of graduate applicants at Rochester more than doubled, resources allocated to graduate students from the College tripled, and the support from research grants nearly doubled. He also started the drive to establish an undergraduate College within the existing University structure. The goal was to focus the attention of the faculty, the students, the administration, and the alumni on the essential significance of undergraduate education. Jack organized extensive discussions through the Faculty Council which ultimately led that representative group to unanimously approve establishment of The College in December 1989.

Jack was one of the most highly recognized and respected members of the Rochester faculty. His insights, enthusiasm, and energy will be sorely missed. His legacy at the University and around the country will live on for many years. We were fortunate to have known him as a colleague, teacher, and friend.

Jack, Prahtiba Varma-Nelson, and David Gosser accepting the ACS Jack Flack Norris Award



Xiaowei Zhuang receives the 2010 Magomedov-Shcherbinina Award

The 2010 Magomedov-Shcherbinina Memorial Prize was awarded to Xiaowei Zhuang on November 9th. This prize memorializes the lives of Nabi, Natalya, and Amir Magomedov who lost their lives in a 2006 multi-vehicle accident. Nabi was a rising assistant professor of the chemistry department. His wife, Natalya Shcherbinina was a research scientist at Bausch & Lomb. This prize is given to a young scientist who has demonstrated exceptional ability in research in the early years of their first independent academic appointment with the promise of outstanding accomplishments in the future.

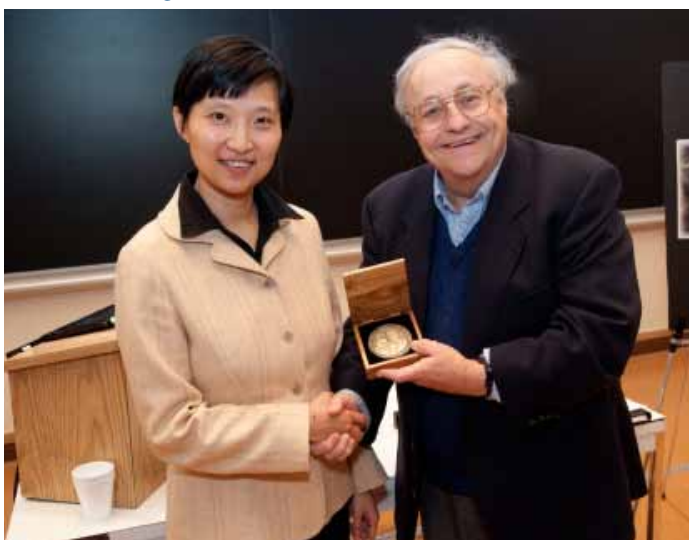
Xiaowei Zhuang lecturing in Lander Auditorium



Xiaowei Zhuang is a professor of chemistry, chemical biology and physics at Harvard University, as well as an investigator at Howard Hughes Medical Institute. She is a leading expert in single-cell biology and bioimaging. With her lab, she develops and applies advanced optical imaging techniques, such as super-resolution light microscopy and single-molecule imaging approaches to study biological systems qualitatively. Zhuang received her B.S. degree in physics from the University of Science and Technology of China, and her Ph.D. in physics from the University of California at Berkeley. In 2001, she joined the faculty of Harvard University as an assistant professor. She was promoted to associate professor in 2005 and full professor in 2006. In addition, Zhuang has received countless awards which include the MacArthur Fellowship, Sloan Fellowship, Packard Fellowship for Science and Engineering, Beckman Young Investigator Award, Searle Scholar award, NSF CAREER award, ONR Young Investigator Award, TR World's Top 100 Young Innovators Award, Camille Dreyfus Teacher-Scholar Award, Coblentz Award, ACS Pure Chemistry Award, and the HHMI Collaborative Innovation Award.

During her stay at the U of R, Zhuang presented a well attended lecture "Nanosopic Imaging of Biomolecules and Cells". This lecture talked about the importance of optical microscopy as a tool in biological research and her development of stochastic optical reconstruction microscopy (STORM). With STORM, Zhuang and her lab were able to achieve multicolor and three-dimensional imaging of molecular complexes, cells and tissue with nanometer scale resolution. The Department of Chemistry was happy to have had the pleasure of hosting Xiaowei Zhuang.

Xiaowei Zhuang with Bob Boeckman



Magomedov Medal on top of Magomedov Memory Book



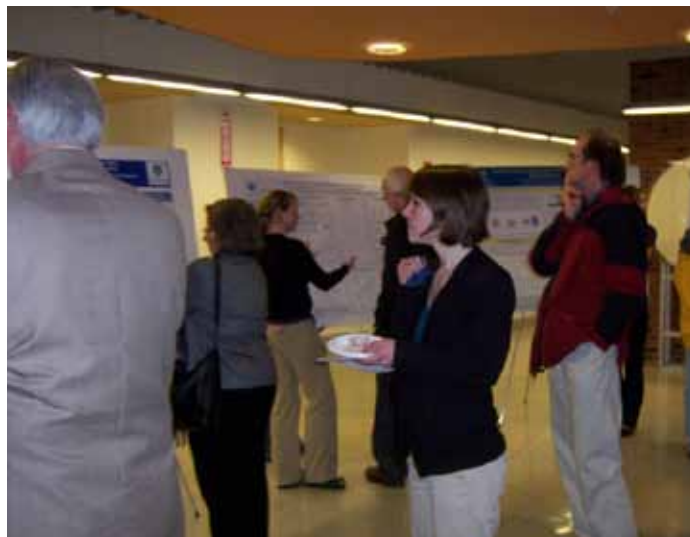
Joseph DeSimone Awarded 2011 Harrison Howe Award

The 2011 recipient of the annual Harrison Howe Award of the Rochester Section of the American Chemical Society was Dr. Joseph M. DeSimone who was presented with this award at the University of Rochester on April 29th. This ACS Rochester Section award was created in 1946 to memorialize one of the founders, Harrison E. Howe. This early career award recognizes an outstanding scientist who has made significant contributions to their field in chemistry and has great potential for more future success. Approximately 40 percent of these recipients have gone on to earn a Nobel Prize in chemistry. The most recent awardee to receive the Nobel Prize was Jack Szostak in 2009 after receiving the Harrison Howe Award in 2003. The Harrison Howe Committee Chair this year was Assistant Professor Bradley Nilsson.

Dr. Joseph M. DeSimone is the Chancellor's Eminent Professor of Chemistry at the University of North Carolina and the William R. Kenan Jr. Professor of Chemical Engineering at North Carolina State University. He has received 40 major awards and recognitions throughout his career and was elected into the National Academy of Engineering, as well as the American Academy of Arts and Sciences, in 2005. He has published more than 260 scientific articles and has more than 115 issued patents in his name, with 120 more patents pending. DeSimone and his group are currently learning how to bring techniques of uniformity, precision, and mass production, associated with the fabrication of nanoscale features found in the microelectronics industry to the nano-medicine field for the production and delivery

of vaccines and therapeutics to treat and prevent diseases. He founded Liquidia Technologies (www.liquidia.com) in 2004, which has about 50 people employed at RTP and has raised over \$30 million in venture financing. DeSimone's laboratory and PRINT Technology are an integral part in the Carolina Cancer Center of Nanotechnology Excellence, funded by the National Cancer Institute.

The 2011 Harrison Howe Reception and Poster Session, Goergen Atrium



Joe DeSimone receiving award plaque from Mitch Anthamatten



Students Breanna Eng and Amanda Chang assisting at the event



Chemistry Welcomes Michael L. Neidig

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

neidig@chem.rochester.edu

Michael's research interests focus on the use of physical-inorganic methods to generate new fundamental insight into structure, bonding and mechanism in non-precious metal catalysis. Michael earned his B.A. in chemistry in 1999 from Colgate University and continued his chemical education as a Winston Churchill Foundation Scholar at the University of Cambridge, earning an M.Phil. degree in chemistry in 2001. He then moved to Stanford University to pursue his Ph.D. in chemistry as an NSF predoctoral fellow with Prof. Ed Solomon. Focusing on mononuclear non-heme iron enzymes, Michael utilized a variety of inorganic spectroscopic methods (magnetic circular dichroism, electron paramagnetic resonance, etc.) to obtain novel insight into structure and activity in a wide variety of systems. These include elucidation of contributions to H-atom abstraction vs. electrophilic attack reactivities in two enzymes with similar active sites, determination of the role of the facial triad in α -ketoglutarate-dependent dioxygenases, and the use of mutants of lipoxygenase to understand the mechanism of this ferric enzyme. After graduation, he moved to the Dow Chemical Company in its Inorganic Chemistry and Catalysis division where his research focused on new catalyst development and mechanistic insight, with a strong emphasis on heterogeneous catalysis. Desiring a return to more fundamental research, Michael joined Los Alamos National Laboratory in 2009 as a Director's Postdoctoral Fellow. His research at Los Alamos spanned several areas including structural elucidation and structure-activity relationships in non-precious metal fuel cell catalysis and highly fluorescent gold nanoclusters. Michael will be contributing to our inorganic chemistry instruction in the fall semester of 2011 and is excited to be teaching CHM 415 (Group Theory) and CHM 425 (Physical Methods in Inorganic Chemistry).

Selected Publications:

Ag K-Edge EXAFS Analysis of DNA-Templated Fluorescent Silver Nanoclusters: Insight into the Structural Origins of Emission Tuning by DNA Sequence Variations. M.L. Neidig, J. Sharma, H. C. Yeh, J. S. Martinez, S. D. Conradson, and A. P. Shreve, *J. Am. Chem. Soc.* **2011**, *133*, 11837-11839.

Direct Observation of Acetyl Group Formation from the Reaction of CO with Methylated H-MOR by in situ Diffuse Reflectance Infrared Spectroscopy. X. Chen, M. L. Neidig, R. Tuinstra, and A. Malek, *J. Phys. Chem. Lett.* **2010**, *1*, 3012-3015.

CD and MCD of CytC3 and Taurine Dioxygenase: Role of the Facial Triad in α -KG-Dependent Oxygenases. M. L. Neidig, C. D. Brown, K. M. Light, D. G. Fujimori, E. M. Nolan, J. C. Price, E. W. Barr, J. M. Bollinger, Jr., C. Krebs, C. T. Walsh, and E. I. Solomon, *J. Am. Chem. Soc.* **2007**, *129*, 14224-14231.

Kinetic and Spectroscopic Studies of N694C Lipoxygenase: A Probe of the Substrate Activation Mechanism of a Nonheme Ferric Enzyme. M. L. Neidig, A. T. Weckslar, G. Schenk, T. R. Holman, M. Kavana, and E. I. Solomon, *J. Am. Chem. Soc.* **2007**, *129*, 7531-7537.

Spectroscopic and Electronic Structure Studies of Aromatic Electrophilic Attack and Hydrogen-Atom Abstraction by Non-Heme Iron Enzymes. M. L. Neidig, A. Decker, O. W. Choroba, F. Huang, M. Kavana, G. R. Moran, J. B. Spencer, and E. I. Solomon, *Proc. Natl. Acad. Sci. U.S.A.* **2006**, *103*, 12966-12973.

Hutchison Hall Gets New Organic Chemistry Lab



The University has created exciting new laboratory space in the chemistry department to teach organic chemistry this fall.

An especially novel feature of the new lab is the incorporation of designed discussion space within the lab. The space will be used to facilitate collaborative students' discussions on the planning, execution and analysis of experiments. The new lab is equipped with modern chemistry instrumentation including a capillary gas chromatograph and two Fourier transform infrared spectrophotometers. The lab was specifically designed and equipped to streamline workflow, allowing students to spend their time in lab more productively. The lab is outfitted with modern multimedia capabilities, including two 70 inch LCD screens, a high resolution LCD projector, and a 10 foot drop-down screen which will allow students to view instructional videos and to display real-time experimental data. The lab also features state-of-the-art "green" fume hoods for students to work in. In addition to creating a safer work environment, the green hoods use high-tech filters to clean and recirculate the lab air, reducing energy costs by as much as 96% relative to conventional (ducted) fume hoods. Additional green features include an in-house vacuum system, which will save tens of thousands of gallons of water each year that would otherwise be used to operate water aspirators, and high efficiency LED lighting.



The 2011 Chemistry-Biology-Biophysics Cluster Retreat

The Chemistry-Biology-Biophysics (CBB) Interface Cluster held its second annual Retreat on June 9-10, 2011. On the afternoon of June 9th, two talks were presented to an audience of about 60 people in Hutchison Hall Room 473. The first talk was “Ferritin Protein Nanocages - How

that is required for healthy growth in yeast.” The third talk, “tRNA molecular dynamics” given by XiaoJu Zhang from the Mathews group, also focused on tRNA modifications, but from a computational approach. The last talk, “Probing the effect of turn nucleation on amyloid self-assembly using β -turn peptidomimetics” by Todd Doran from the Nilsson group provided insight into protein folding related to Alzheimer’s disease.



Amy Ensign, Jake Yeston, Corine Farewell, Rudi Fasan (top left to right); Kara Bren, Doug Turner, Elizabeth Theil, Sachdev Sidhu (bottom left to right)

Iron Moves In, Out & Controls Biosynthesis” by Elizabeth Theil, Senior Scientist at Children’s Hospital Oakland Research Institute (CHORI). The second talk was “Synthetic Proteins: New Tools for New Biology” by Sachdev Sidhu, Associate Professor of Molecular Genetics at the University of Toronto. Professor Sidhu arrived in the middle of Dr. Theil’s talk after being held up at the border for two hours. Apparently, the border agents did not believe that he would drive from Toronto to Rochester to present a lecture for free. Both talks highlighted methods ranging from molecular biology to crystallography and the results had clear implications for medicine.

The Retreat reconvened in the Munneryn Atrium in Goergen Hall on the River Campus at 9:30 AM the next day with 80 attendees. The day started with fruit, juice, coffee and breakfast pastries and a session of 22 posters ranging from synthesis to computations, with a wide variety of studies in between. This was followed by a buffet lunch, four scientific talks, and a very animated and informative Career Panel Discussion. New Chemistry Professor, Oleg Prezhdho, introduced the audience to a new way of thinking about intermolecular interactions by discussing “The Catch Bond – Where is the Catch?” Dr. Michael Guy from the Phizicky group next took the audience to another side of the CBB Interface with his talk on “2’-O-methylation of residue C32 of phenylalanine tRNA is the only modification of the six catalyzed by highly conserved Trm7

The hour long Career Panel Discussion was held between the second and third talks. The panelists were Elizabeth Theil, Sachdev Sidhu, Corine Farewell (Director of Office of Technology Transfer, University of Rochester), Amy Ensign (Assistant Professor of Chemistry, Roberts Wesleyan College), and Jake Yeston (Senior Editor, *Science*, AAAS - American Association for the Advancement of Science). The panelists described their experiences in a wide range of environments. For example, Dr. Theil was an endowed University Professor at North Carolina State University before moving to CHORI; Professor Sidhu worked at Genentech for about a decade before moving to academia; Dr. Farewell has D.V.M. and M.B.A. degrees from Cornell and worked in Germany for a Proctor & Gamble subsidiary before moving into management of academic intellectual property; Professor Ensign was a graduate student with Kara Bren until she took her faculty position two years ago; Dr. Yeston was a postdoc in Germany before joining *Science*. As usual, a common theme of the discussion was that careers rarely go in a direct line and that it pays to be flexible and to take advantage of opportunities that may arise by accident. Another major theme was ways to balance career with family life. More than one way was suggested. The discussants gave interesting and candid answers to questions and inspired the audience to think about their own career plans.

This year’s Retreat included posters and speakers from the Departments of Biochemistry & Biophysics, Chemistry, Microbiology, and Pediatrics. 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 the Department’s summer Research Experience for Undergraduates program. The Retreat gave all participants a broad overview of research related to biology and medicine and an appreciation of interdisciplinary approaches.

Student Awards and Accolades



Karen Chiang's "Chemistry Thought Bubbles"

Record Number of NSF Graduate Fellowships

LAURA ACKERMAN (1st-year grad student, Weix Lab), **ALEXANDER FEDERATION (B.S. '11)**, Nilsson Lab), **CAITLYN ROSE KENNEDY (B.S. '11)**, Frontier Lab), and **RANDY SABATINI** (2nd-year grad student, McCamant and Eisenberg Labs) were announced as 2011 National Science Foundation Graduate Research Fellows on April 5th. Recent graduate **RANDY MEHLENBACHER (B.S. '10)**, currently in the chemistry graduate program at the University of Wisconsin, also earned an award. **PETER CARLSEN** (2nd-year grad student, Frontier Lab), **KIMBERLY MANBECK** (1st-year grad student, Jones Lab), and **DAVID WEINBERG (B.S. '11)**, Rothberg Lab) were listed as honorable mentions. "This is an exceptional group of students," noted Assistant Professor Daniel Weix, who also attributed the department's recent success to increased encouragement for competitive students to apply. Congratulations to all the awardees!

C&EN Photo Contest

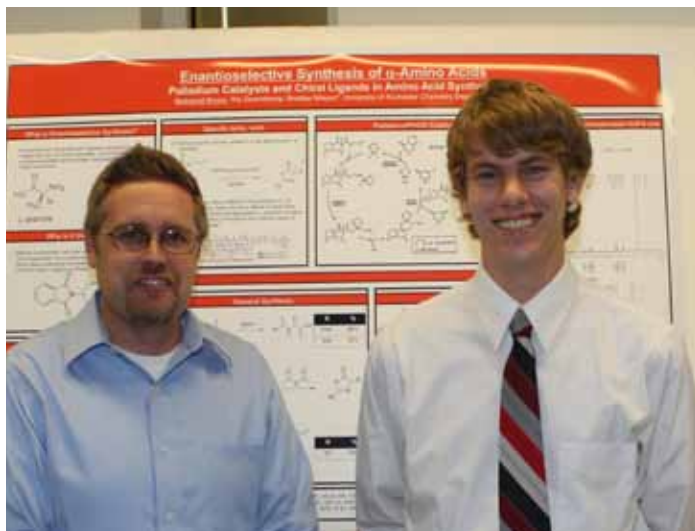
The Chemical and Engineering News (C&EN) asked readers to submit photos on all things chemical, giving them the broad theme of "Your Science Up Close". The submitted

photos, with a count of almost 250, ranged anywhere from the everyday science observation to a reaction that was never expected to happen. **KAREN CHIANG**, a grad student in Pat Holland's lab, received honorable mention for her photo (shown above) entitled "Chemistry Thought Bubbles". The picture was taken of a book titled "Nontraditional Careers for Chemists" by Lisa M. Balbes, through a glass of water containing air bubbles.

Randy Sabatini and Laura Ackerman



ALEXANDER FEDERATION (B.S. '11), received the 2011 ACS Rochester Section Award and a National Science Foundation (NSF) Graduate Research Fellowship to help him further his studies in chemical biology at Harvard this fall. After a summer working at the Johns Hopkins Institute for NanoBiotechnology in 2009, he came back to Brad Nilsson's lab and began working



Brad Nilsson and Alexander Federation

on finding small peptides to bind to β -amyloid, the misfolded protein implicated in Alzheimer's disease. Outside of the lab, Alex was a workshop leader for several different chemistry and biology courses and also devoted time to running as part of the University of Rochester cross country and track teams.

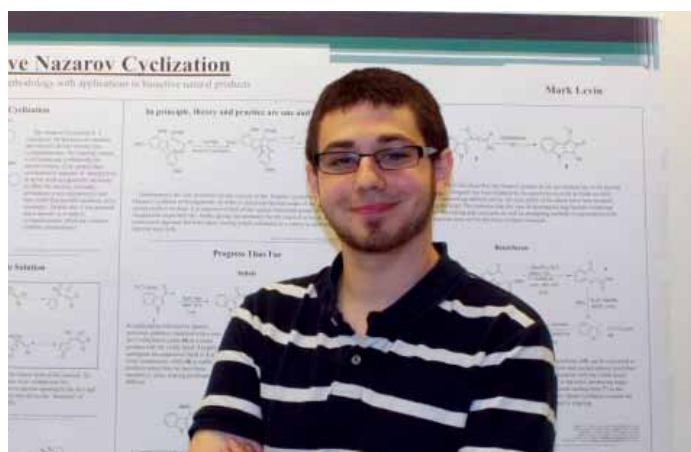


CAITLYN ROSE KENNEDY (B.S. '11), was also awarded an NSF Graduate Research Fellowship to pursue her Ph.D. in chemistry, which she began this fall at Harvard. She is also the second chemistry major in two years to have received both the Catherine Block Memorial (junior woman) and Janet Howell Clark

Prizes (senior woman). Last year Rose was awarded the Gladys Anderson Emerson Scholarship funded by Iota Sigma Pi, which is given to a woman in her third year of undergraduate studies for excellence in chemistry or biochemistry. She received the John McCreary Memorial Prize at graduation. Rose worked on her senior thesis research with Professor Alison Frontier on the development of the Morita-Baylis-Hillman-like Nazarov Cyclization. She also served as a workshop leader for several chemistry courses during her years here, receiving the 2011 Carl A. Whiteman, Jr. Teaching Award.

Rising senior **MARK LEVIN**, received the 2011 ACS Inorganic Chemistry Award. He also received an honorable mention as a 2011 Barry M. Goldwater Scholar, the fifth student from the

University of Rochester to receive this distinction. The Goldwater Scholarship, which is endowed by the U.S. Congress in honor of the late Sen. Barry M. Goldwater, is a competitive fellowship for undergraduate students in science, math, and engineering. The scholarship is worth up to \$7,500. Each year, 10 to 20 sophomores and juniors compete for the four University nominations to the national competition of 1,100 candidates. Applicants must rank in the top quartile of their class while demonstrating outstanding research skills, potential for advanced study in their fields, and a strong commitment to pursue research-oriented careers. Mark, of Cleveland, Ohio, will graduate next year with a bachelor of science degree in chemistry and a minor in mathematics. He spent the 2010 summer participating in the German Academic Exchange Service-Research Internships in Science & Engineering Scholarship (DAAD-RISE) program. While in



Mark Levin

Germany, he worked in an organic chemistry laboratory at the Technical Institute of Braunschweig. This spring, Mark was named an Amgen Scholar, which helped fund a summer research experience with the Toste Group at the University of California at Berkeley. An ambassador for Rochester, Levin works as a Meridian in the University's Office of Admissions, leading campus tours for prospective students. He also is a member of the Undergraduate Chemistry Council and serves as a resident advisor for the Office of Residential Life and Housing Services. Levin plans to earn an advanced degree in chemistry after graduation.

Each year, the University awards the Catherine Block Memorial Fund Prize to a woman in the junior class in recognition of her outstanding ability and achievement in the field of science.

This year, chemistry major and Rochester Early Medical Scholar (REMS) student **EMILY REDMAN** received the CBMF Prize. Emily spent her summer in Thailand, one of seven United States students to



participate in a joint Research Education for Undergraduate (REU) program with the University of California – Santa Cruz and Chulalongkorn University, Mahidol University and the Chulabhorn Research Institute. Students took part in a group research effort in organic chemistry after a short course on Thai language and culture was provided.

The Edward Peck Curtis Award for Excellence in Teaching by a Graduate Student is a University wide competition given to exceptional teaching assistants. **JOHN FROST** was among five graduate students across the University who received the 2011 award. The nomination includes letters of support from the chair, faculty and students. The recipients were honored at a luncheon with the provost and dean of graduate studies.

This year the chemistry department fielded two softball teams. The incumbent chemistry department softball team, “Hutch’s Hitters”, coached by **MICHAEL PRINSELL** and **MATT BETUSH**, made a trip to the playoffs for a third consecutive year. The team was comprised of many returning members of last year’s 2nd place finishing team (professors, graduate students and spouses) along with several new younger students (both graduate and undergraduate). Shortstop **ERIC HENRY** (.867) and left center fielder **DAN EVERSON** (.778) led the team in hitting, on the way to a 6-2 record and the 3rd seed in the playoffs. Unfortunately, strong pitching from Professor Boeckman was not enough to power the “Hitters” past “University IT” resulting in a 5-2 playoff loss. The coaches would like to thank the team for another strong season. Hopefully we can return to the playoffs for a fourth year in 2012.

Hutch’s Hitters defectors **RANDY SABATINI** and **STEVE JACOB** started an expansion team, The Sheridan Shamrocks, who had a fantastic season...not on paper, but in spirit. Every game saw improvement and an increasing cohesiveness that resembled the formation of a polymer. The final game of the season, aptly named “The Miracle on Field 5,” was one of, if not the greatest game of softball ever played on Field 5. The halls of Hutchison will resonate with the cheers of the players for years to come. It was billed as the “battle of last place.” Both teams winless and out for blood. Our team was riddled with injury; torn MCL, broken toe, stress induced migraines from an oral exam; we had them all. The opposing team was significantly older and wiser, it seemed we hadn’t a chance. Amazingly, **KYLE BIEGASIEWICZ** pitched a nearly perfect game. Our injured star outfielder, **SHAUN SHAHAN**, mustered up the courage to stand at the plate with his MCL nearly hanging off his leg and go 2 for 2 at the plate, **KELLY SOWERS** and **KIM MANBECK** both had RBI’s and **YU-WEN HUANG** laid out like superman to catch a line drive. Everyone seemed to be glowing with talent that night and lo and behold, we prevailed. A great man once said in a dream, within a movie, “heros get remembered, but legends never die.” In the coming seasons we will hopefully have more wins and continue to improve, but not one of us will ever forget the Miracle of Field 5.

[See Also Commencement Awards on p. 66](#)

The two chemistry softball teams, Sheridan Shamrocks on left and Hutch’s Hitters on right



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 2010-2011 academic year, **ROBERT K. BOECKMAN, JR.** completed his eighth year as the chair of the chemistry department. Professor Boeckman is continuing as chair for the 3rd year of a 3-year term in 2011-2012. He also continues his duties as associate editor of the *Journal of Organic Chemistry*, and as vice president and member 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 hydroxy-methylation of aldehydes. Studies in this area are continuing

Rush Rhees Library



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 Department of Pediatrics URMC whose goals are 1) the identification of the biological target(s) of a novel series of small molecules which mimic the effects of caloric restriction on lifespan in yeast and in small mammals and 2) the development of 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) defended his thesis and continues as a postdoctoral associate in the group working on the Goldfarb (biology) collaboration. **JOHN R. MILLER (PH.D. '10) AND YAN MILLER (PH.D. '10)** defended their theses in March of 2010 and moved on to Stanford University, where they both began work as postdoctoral associates in Barry Trost's group. John will join the law firm of Hodgson Russ LLP in Buffalo, NY in July 2011 as a scientific advisor and Yan Miller is currently seeking employment in the Buffalo area. **NATHAN E. GENUNG (PH.D. '10)** continues as a postdoctoral associate with Larry Overman at UC Irvine. **XINYI SONG (PH.D. '07)** was married in July 2011 and is currently employed as a research chemist with J&W Pharmed in Levittown, PA. Matt Betush continues his research in the group on various aspects of asymmetric catalysis. George Arab and Brian Ohman are completing their 4th year and continue working on FK-506 and Apoptolidin, respectively. Part-time scientist Dr. Dennis Savage, retired from Kodak, continues his work in



Meliora Medallion

the group on several projects with the Goldfarb (biology) and Krysan groups (pediatrics URMC). **CHRISTOPHER WONG (B.S. '11)** completed his B.S. thesis in the group in Spring 2011 and will begin graduate studies in chemistry at Boston University in the fall. During the summer of 2010, one undergraduate worked in the group as part of the NSF REU program along with two new graduate students, Doug Tusch from RIT and Kyle Biegasiewicz from Niagara U. Both joined the group permanently in December 2010. Doug and Kyle are collaborating on an organocatalysis project and helping out with FK-506 and Apoptolidin when time allows. David Kaphan, a UR senior, has worked in the group since his freshman year and will do his B.S. thesis in the group during the 2011 academic year after having spent the summer of 2010 working at Novartis in Cambridge, MA. Two new graduate students Gil Ryenders (Lake Forest College) and Adam Feinberg (RIT) and three undergraduates, Wil Ksander (Beloit College, WI), Emily Vogt (Ohio U.), and Peter Jaenike (U. Buffalo) are working in the group during the Summer of 2011. **CHRISTINA COLLISON (PH.D. '04)** recently was promoted to associate professor with tenure in the chemistry department at RIT and **JEREMY CODY (PH.D. '04)** continues as assistant 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)** recently joined AstraZeneca in Waltham, MA as research scientist.



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 had a busy year pursuing projects in heme protein structure-function relationships, in protein folding, and in solar energy conversion. A highlight was celebrating the graduation of **SARAH BOWMAN (PH.D. '10)**, who left for her postdoc at MIT with Professors Cathy Drennan and Collin Stultz. We also were thrilled to hear Sarah's recent news that she was awarded an NIH Postdoctoral Fellowship.

The studies of cytochrome electronic structure and function have moved forward well, led by postdoc Matt Liptak and graduate students, Jesse Kleingardner and Mehmet Can. Matt published an interesting paper in *JACS* reporting the effect of interactions with heme propionates on electron transfer activity and on pro-apoptotic activity of human cytochrome *c*. Jesse also had a publication in *Metallomics* on the requirements for heme attachment in mitochondrial cytochromes *c*. He is following up that result by performing studies of the conformation of the heme in cytochromes

with unusual modes of heme attachment with the assistance of incoming first-year graduate student Rebecca Smith. Mehmet Can has new results linking heme conformation to its EPR spectrum in collaborative work with Prof. Kristofer Andersson (University of Oslo) now submitted for publication. Mehmet is also studying high-spin cytochrome *c* variants with the assistance of U of R undergraduate Ben Snyder, who is doing his senior thesis project in the Bren lab. Jesse and Mehmet gave talks on their results in a symposium on heme modification and regulation at the ACS National Meeting in Anaheim (March, 2011). Jesse won a travel award from the ACS Division of Biological Chemistry to present this work. In summer 2011, Matt will be departing for a faculty position in the Department of Chemistry at the University of Vermont. We will miss his contributions to the project but are thrilled to see him strike out on his own.

The group's efforts, pursued jointly with the Krauss group, to study cytochrome *c* folding on the single-molecule level

Carlson Library and Computer Studies Building



have continued to move forward. Postdoc Andrea Lee and graduate student Wesley Asher have exciting new data. Wes won a travel award from the ACS Division of Biological Chemistry to present his results at ACS in Denver (August, 2011), and Andrea was invited to present her results at the 2011 Aspen Meeting on Single Molecule Biophysics where she was the only non-faculty member to give a talk. Wes also has continued to pursue his work on heme-tagged proteins with the assistance of UR undergraduate Emily Redman. We congratulate Andrea who will be taking a research position at the University of Vermont starting this summer.

The Bren group is continuing our efforts to develop porphyrin peptides for energy conversion in a collaborative project with the Eisenberg, Holland, and Krauss groups. The two new members who joined the group this year are focusing on this project. First-year student Shaun Shahan joined as a joint student with the Krauss lab and is developing porphyrin peptides for use in photoinduced charge transfer. He also is utilizing fluorescent zinc-substituted cytochromes to probe intermolecular interactions and, with the assistance of NSF-REU student Lisa Richter from Luther College, expressing a photosynthetic cytochrome *c* for further study. In addition, Anni Siitonen, a postdoc joint with the Krauss lab who also started in the past year, is engineering porphyrin-



Interfaith Chapel



nanotube structures for long-range photoinduced charge transfer. Graduate student Lenore Kubie, also a Bren/Krauss joint group member, is studying protein-nanotube and peptide-nanotube interactions. Lenore is supported by an NSF IGERT grant in Distributed Renewable Energy and this summer is pursuing an internship at the National Renewal Energy Lab (NREL) in Colorado. Finally, Erin Knappen-Kleingardner is continuing her development of heme peptide expression and is writing her first manuscript resulting from the work. Erin and Anni also are mentoring an incoming biophysics student, Tom Hilimire, who is conjugating cytochromes and quantum dots for charge transfer. The group is enjoying seeing this work develop as we expand the collaborative aspects of the project.

A group alumnus, **LINGHAO ZHONG (PH.D. '03)**, informed us that that he has been awarded tenure at Penn State Mont Alto, making him the first graduate of the Bren lab to receive tenure. Although this news makes Kara feel old, she was thrilled to hear of his continued success.

Kara had another busy year, taking on the directorship of the Biological Chemistry Cluster and also chairing the Graduate Recruiting Committee. She also organized a symposium on Heme Modification, Transport, and Regulation at ACS in Anaheim (March 2011) along with Prof. Eric Hegg of Michigan State. This past year saw a lot of travel for Kara who gave invited talks at five conferences as well as at seven colleges and Universities.



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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An interesting finding obtained in our recent simulations for DNA with the code CP2K was the rapid contraction of a hole injected into the DNA. Immediately after injection, the hole wavefunction was spread over 5 adenines, the extent of the QM region. Within 20 to 25 femtoseconds the wavefunction was almost entirely contained on a single adenine. At 300K, the hole stays on this adenine for the length of the simulation, typically a few hundred femtoseconds. We considered three possible reasons for the contraction: (1) An electronegative nitrogen on adenine (N7 or N3) forming hydrogen bonds with water and in the process repelling the hole from all but one adenine; (2) a concentration of water molecules around one adenine, forming a stable region for the hole; (3) polarization of the surrounding water by the positive charge of the hole.

Carrying out our simulation, we found that, around the adenine with the hole, during the time the wavefunction contraction was taking place, the closest water molecules were still at least 4Å away, a distance too great to allow the formation of a hydrogen bond. With time, diffusion brings water molecules closer to the adenine with the hole, but the earliest any appropriately oriented water molecule is seen to come within bonding distance is ~ 150 fs, well beyond the time scale in which the contraction occurs. The finding of such a low concentration of water near the adenines also rules out the possibility of the contraction mechanism being the elimination of the hole wavefunction from all but one adenine by the formation of hydrogen bonds between the electronegative nitrogens and water hydrogens on all the other adenines.

We found several types of evidence that the polaron contraction is due to the polarization of the water by the hole. The very short time required for the polarization can be attributed to the very rapid librational motion of the water, which allows correspondingly rapid rotation of the water dipoles. The time dependence we found for the size of the hole is consistent with there being two different librational modes with different frequencies, as is known to be the case for water. We showed also that localization

of the hole on a single site led to the lowest energy of the system. Our work is significant in establishing that the steady state hole wavefunction, rather than extending over several adenines, is localized on one, a proposition that is still being debated by those working in the field.

Esther enjoyed working with her two undergraduate students: **COLIN KINZ-THOMPSON (B.S. '10)** who went on to Columbia for graduate studies, and Shane Kravec who is currently a senior in physics.



Esther with student Shane Kravec



RESEARCH INTERESTS

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

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JOE DINNOCENZO and his group continue to pursue a variety of problems in photoinduced electron transfer and related chemistry. As part of an ongoing collaboration with Samir Farid, we discovered that ground state electron transfers between neutrals and cation radicals have a rate constant/driving force dependence that surprisingly follows a simple Sandros-Boltzmann dependence. We also found that the charge shift, electron transfer quenching of excited pyrylium cations by neutral donors also had the same dependence. Most surprisingly, we found that excited state quenching of neutral cyanoaromatics by neutral electron donors had a Sandros-Boltzmann dependence on the driving force for electron transfer. Our results contrast with the well-known Rehm-Weller description of excited state electron transfer quenching (k_q) involving neutral donors and acceptors ($A^* + D \rightarrow A^{\cdot-} + D^{\cdot+}$), where a gradual fall off in $\log k_q$ vs ΔG is reported. This caused us to carefully reexamine all of the original Rehm-Weller data. Remarkably, when accurate redox potentials are used for the electron donors and acceptors, and when one excludes data points in the highly endergonic region that are not due to electron transfer, the quenching constants for the experiments described by Rehm and Weller were found to follow a Sandros-Boltzmann dependence on driving force! Perhaps more important from a mechanistic perspective, all of the reinvestigated Rehm-Weller reactions were found to proceed through exciplex intermediates. Historically, the Rehm-Weller reaction and numerous other similar reactions have been quantitatively modeled with electron transfer theories that all assume one-step complete transfer of an electron from a donor to an acceptor in contact. This is not the mechanism of the Rehm Weller reactions, which involve partial electron transfers from A^*/D to the exciplex and from the exciplex to $A^{\cdot-}/D^{\cdot+}$. Thus, it seems likely that our results will lead to the reinterpretation of a large body of previously published data, and will require the development of new theories to fit partial electron transfer reactions.

During the past year we have also solved a long standing puzzle in cation radical reactivity, namely understanding the unusual chemistry of aryltrimethylstannane cation radicals, which are unique amongst known Group 14 cation radicals in that they undergo Sn-C bond fragmentation to preferentially give the less stable aryl radical rather than a methyl radical. Our experiments show that the stannane cation radicals fragmentations are not unimolecular, as previously thought, but are nucleophile-assisted. This new reaction mechanism can readily explain the otherwise perplexing chemistry of these stannane cation radicals. Along similar lines, the group also continues to investigate new aspects of organosilane and organogermane cation radical chemistry.

Joe is also enjoying a pedagogical research project to introduce Peer Led Team Learning (aka Workshops) into CHM210 (Honors Organic Laboratory II). Joe is working with graduate student Terrell Samoriski, whose Ph.D. studies will involve design of the Workshop program and evaluation of its impact.

Campus Winter Scene



Richard Eisenberg

Tracy H. Harris Professor of Chemistry

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

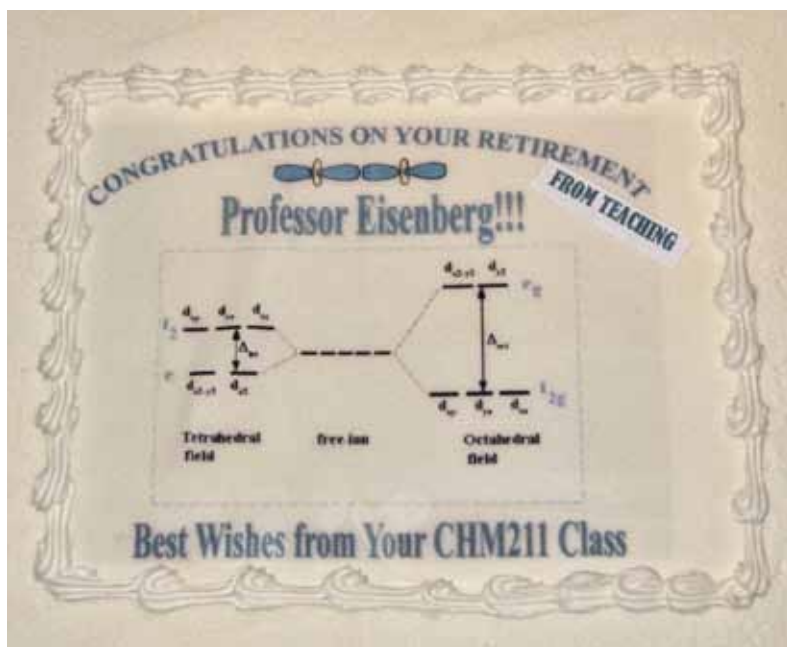
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Another momentous year and one that **RICH EISENBERG** was happy to share with past and present students, colleagues and friends at "Richfest" in May. The celebration in honor of Rich's career (see p. 16) also marked a transition from full-time faculty member to research professor. Rich's formal teaching ended in the Fall 2010 semester with CHM 211, Advanced Inorganic Chemistry, an upper level undergraduate course he has taught for many years. The final lecture was marked with a student-designed cake and a champagne toast. While Rich loves the course and its material, he is also happy with no more tests and grading. Formal teaching aside, Rich and the Eisenberg group remain active and vigorous in the pursuit of science.

In July 2010, Rich was a plenary lecturer at the International Conference on Coordination Chemistry in Adelaide, Australia. The trip afforded Rich and Marcia the chance to snorkel on the Great Barrier Reef, see kangaroos, wallabies and koalas in the wild, and enjoy the beauty and vibrance of Sydney. After several trips to the west coast in January for the annual ACS Editors meeting and the NSF Center for Chemical Innovation on Solar Fuels (Rich is a Scientific Advisory Board member), the

activities in 2011 ramped up. In March at the ACS Meeting in Anaheim, former student Pingwu Du and Rich were honored with the ACS Nobel Laureate Award for Graduate Education. The award symposium featured talks by Dan Nocera, **CLIFF KUBIAK (PH.D. '80)**, Phil Castellano and Harry Gray, in addition to the award address given mainly by **PINGWU DU (PH.D. '09)**. Interesting science and great fun was enjoyed by all. Also at the meeting, Rich participated in other symposia honoring long-time friends Alan Balch and Pete Wolczanski who were also award recipients. In April, Rich was formally inducted into the National Academy of Sciences, "one of the highest honors to which we can aspire." The induction ceremony was attended by Rich's immediate family. The subsequent NAS annual meeting included talks and workshops (Rich moderated one on sustainable energy), and ended with a black-tie ball (great music and dancing). In May, there was the special "Richfest" celebration, and the day after it was over, Rich and Marcia were off to Prague for a Conference on Solar Fuels, after which they journeyed to Florence and the Cinque Terra for vacation. For the latter, they met up with Maurice Brookhart and his wife to hike from town to town in one of the most charming locales

Rich & Marcia at the National Academy of Sciences Award meeting with family and friends



they have ever visited. The wine and food were great too! After Italy, Rich continued his travels onto Israel where he is chairing a committee of the Council for Higher Education to evaluate chemistry programs and research for all institutions which grant Ph.D.'s in Israel. The trip lasted 12 days with another planned in December. After returning home in late June, Rich returned to Europe a week later for the International Symposium on the Photochemistry and Photophysics of Coordination Compounds in Strasbourg, France, where he was a plenary lecturer. Rich reflects that this is hardly what he thought his transition would be - he now calls it "refirement."

This year marks the 50th volume of *Inorganic Chemistry*. The journal is doing well with special events planned to commemorate the golden anniversary year. One of these is a special symposium to be held at the ACS Meeting in Denver in August, while another is a series of interviews hosted by Rich that are on the web with leaders in the field (<http://pubs.acs.org/page/inocaj/multimedia/voices.html>). The interviews have been well received with favorable comments coming in from all over the world. Rich says the interviews are best enjoyed with a glass of wine and some time to ponder why chemists do what they do. He is especially gratified by teachers who say they will use the interviews in their courses (without the wine). Rich is also deeply appreciative of the tireless efforts put in by Arlene Bristol, Kirstin Campbell and spouse Marcia in the Editor-in-Chief's office, as well as by the Associate Editors, their assistants, and the many staff who keep the journal running so successfully.

The Eisenberg group continues to make progress developing and analyzing new systems for the photogeneration of H₂ from

water which is the reductive side of water splitting and one of the key reactions for light-to-chemical energy conversion. Research on this problem is spear-headed by postdoctoral researcher Bill McNamara and graduate student Zhiji Han. Both Bill and Zhiji are co-advised with colleague Pat Holland under a DOE grant to Kara Bren, Todd Kraus, Pat Holland and Rich for a multi-pronged approach to the solar hydrogen challenge. 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 for H₂ generation. On iridium catalysis of electrocyclization reactions in a joint project with Alison Frontier, several articles were published on research by graduate student Tulaza Vaidya who has made presentations at the last two ACS Meetings and continued her streak in Denver in August.

Group comings and going for the year include the departure of postdoc Theresa McCormick who did wonderful research for two years as an NSERC Fellow on the photogeneration of hydrogen and the arrival of postdoc Will Eckenhoff from Duquesne who will also work on this problem. Undergraduate researcher Paul Alperin also carried out a notable senior research project and will start Ph. D. studies this Fall at Stanford University. Finally, as this article is being written, Jerry Manbeck, Rich's last solely advised graduate student, has defended his thesis on new luminescent Cu and bimetallic Cu/Au complexes, including an impressively bright one that contains a steroid derivative as a ligand. Jerry will be leaving shortly to assume a postdoctoral research position at Virginia Polytechnic Institute with Professor Karen Brewer.

Rich with students in his last class, Dec 2010



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. Rate constants for thermal and photochemical electron transfer reactions were found not to follow a model that has been universally accepted for over 40 years. Instead, the new data, published in two papers in *JACS*, showed that the rate constants follow a simple Boltzmann-type dependency on the reaction free energy. Thanks to cur-

rent work by Pu Luo, an exceptional graduate student in Joe Dinnocenzo's lab, the scope and limitations of the new model have been significantly expanded. For example, we now know that steric hindrance has a profound effect on thermal electron transfer reactions.

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.

CONTACT

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JIM FARRAR continues to study low energy ion-molecule reactions, with special emphasis on ion-radical reactions using imaging techniques. He has been joined by postdoctoral fellow Linsen Pei, who received his Ph.D. degree from the University of Science and Technology of China, and most recently worked with Professor Chunlei Guo in the Institute of Optics. Linsen's superb experimental skills have been vital in bringing the new detection system up to speed.

Jim continues to work with the Kearns leadership center, along with the Office of Minority Student Affairs, to provide academic assistance to minority students interested in pursuing careers in science. This activity, supported by several dedicated, talented graduate students, has established a strong connection between Chemistry and University efforts to support minority student success in the sciences. Earlier this year, an

NSF S-STEM grant for \$598,000, for which Jim served as PI along with Beth Olivares from the Kearns Center, was awarded to the University in support of this work.

With support and encouragement of our late colleague Jack Kampmeier, Jim introduced Peer-Led Team Learning (PLTL) workshops into freshman chemistry over a decade ago. Based on the success of that initial effort, PLTL workshops have become an integral component of all of Jim's teaching. He has enjoyed working with many talented undergraduate and graduate student workshop leaders, and has particularly enjoyed collaborating with Dr. Catherine Perez from the Center for Teaching and Learning to help leaders become more effective peer mentors. The large number of students who volunteer to be workshop leaders is a strong testimony to the success of the program.

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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It has been a productive year for the **FASAN** group with a series of important achievements being realized in the lab, both in our P450-centered projects and within our efforts directed at constructing and evolving macrocyclic organo-peptidic structures for targeting protein-protein interactions. The year started well with a paper by post-doc Kaidong Zhang and UR undergraduate and McNair fellow Shady El Damaty being published in *Journal of the American Chemical Society*. This work introduced a method for mapping the active site of cytochrome P450s ('P450 fingerprinting') in order to rapidly assess and predict the reactivity of these enzymes. We found that through analysis of the P450 fingerprints, reliable predictions can be made regarding the catalytic activity of these enzymes toward substrates structurally related to the fingerprint probes and information can be obtained also regarding their regioselectivity properties. The group is currently investigating the potential of P450 fingerprinting and fingerprint analysis to enable the engineering of P450 C-H oxidation catalysts with tailored regio-

and stereoselectivity, with first exciting results being obtained both in the context of the antimalarial artemisinin and the anticancer parthenolide. In the artemisinin project, Kaidong has been joined during the year by two talented UR undergraduates, Brian Shafer and Matthew Demars II. First-year graduate student Josh Kolev joined the group this year and he has been focusing on P450-mediated oxidation and chemoenzymatic functionalization of parthenolide, getting off to a great start in this project, which involves a collaboration with Professor Craig Jordan at the UR Medical Center.

During the past year, we also had a series of breakthroughs in our efforts toward developing chemo-biosynthetic strategies for generating macrocyclic organo-peptide hybrids. A first paper in this area, coauthored by Jessica Smith (third-year student) and Francesca Vitali (postdoc), appeared in *Angewandte Chemie* earlier this year and it was highlighted as a "Hot paper" in the same journal. UR undergraduate and McNair fellow Steven

Fasan Group, Summer 2011



Archer also contributed to the project. In a parallel study, Maragani Satyanarayana (postdoc), Francesca, and John Frost (second-year student) were successful in developing a highly efficient and catalyst-free method for constructing organo-peptide macrocycles via an oxime/intein-mediated dual ligation, which will be published in *ChemComm*. Building on these studies, John and his valuable undergraduate collaborator Nick Jacob succeeded in developing a strategy for synthesizing lariat and cyclic peptides in living bacteria cells, while another milestone was achieved by Jessica by implementing a bacterial display system for ultrahigh-throughput screening of our macrocyclic ligands against protein targets. John completed his second year oral exam in July and his outstanding performance as teaching assistant for CHM131 and CHM207 was recognized with a Walters Teaching Award in 2010 and the Peck Curtis Award earlier this year.

Other exciting news concerns the influx of funds to support the group's research. In spring, Rudi was selected as a recipient of the 2011 Provost's Multidisciplinary Research Award along with Prof. Craig Morrell (School of Medicine and Dentistry) and Prof. David Goldfarb (Biology) for a collaborative project related to the synthesis and bioactivity evaluation of chemoenzymatic artemisinin derivatives. The group was also awarded a grant from the National Science Foundation, which will support a three-year project aimed at developing and investigating macrocyclic organo-peptide ligands for selective recog-

nition of oncoproteins Hdm2 and HdmX and disruption of their interaction with tumor suppressor p53.

The group has welcomed a number of motivated and enthusiastic UR undergraduate students to the lab this year: Brian Shafer, Matthew Demars II, Yick Chong Lam, Micah Brown, and Hojun Lee, who have helped in a variety of synthetic and protein engineering projects. Matt and Yick will continue work through the summer of 2011, with Matt being supported by a De Kiewiet fellowship from UR Department of Biology and Yick receiving support from the REU program. Jabari Henriques from North Carolina A&T State University will also join us for the summer as McNair Summer Research fellow. **JACQUELINE ZAENGLE (B.S. '11)** graduated in May, receiving the Merk Index Award in recognition of her academic and research accomplishments. Jacqueline carried out a senior thesis research project in the lab studying the effect of unnatural amino acid incorporation on P450 function. Rajesh Ravikumar, who worked elbow-to-elbow with Jacqueline on this project, will start graduate school at Carnegie Mellon in the fall. Shady El Damaty and Steven Archer, two former members of the group, will join the graduate program at Drexel University. Finally, the group wishes best of luck to **MARAGANI SATYANARAYANA (POSTDOC '10)**, who moved to a post-doctoral position at the University of Massachusetts Lowell.

Statue of George Eastman on the Eastman Quadrangle



Alison J. Frontier

Associate 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. The study of Nazarov cyclization continues, as more and more variations on the cyclization are uncovered. The development of rearrangement chemistry gets more and more interesting, as have efforts to discover alternative starting points for the 4π electrocyclicization. Work on asymmetric cyclizations and applications of Nazarov cyclization toward total synthesis of natural products continues. The study of diastereoselective hydrogenation of pyrroles is also underway, as well as efforts toward the synthesis of the natural products phomactin A, and cyanthawigins U and AC.

Tulaza Vaidya (fourth-year student, working jointly with Rich Eisenberg) has developed remarkably active Ir(III) complexes as Nazarov cyclization catalysts. This year she discovered and developed a new reaction pathway of furans and benzofurans, that only occurs using the reactive Ir(III) complexes. We continue to study rearrangement chemistry that occurs during Nazarov cyclization (Eric Theiste, fourth-year student; and Dr. David LeBoeuf), which is not only stereospecific but also highly che-

moselective in most cases. The products have adjacent stereocenters, and also adjacent quaternary centers. Two additional interesting versions of the Nazarov cyclization were developed in the group this year: Bill Spencer (third-year student) studied initiation of Nazarov cyclization by oxidation of vinyl alkoxyallenes, and Josh Brooks (third-year student) has developed efficient Nazarov cyclization initiated by addition of nucleophiles to unsaturated diketones. All three of these variations give cyclopentane-containing products that are quite different from the cyclopentenone products of conventional Nazarov cyclization. Steven Jacob is continuing to develop methodology for the synthesis of complex pyrrolidines via diastereoselective and enantioselective hydrogenation of pyrroles,

In our natural product synthesis studies, Jen Ciesielski (fourth-year student) is getting closer and closer to the bridged oxadecalin structure of phomactin A, and Peter Carlsen (second-year student) has built a tetracyclic precursor to tetrapetalone A using interesting and efficient chemistry. Yu-Wen Huang is working on a streamlined and enantioselective synthesis of the potent antiproliferative roseophilin.

Frontier Group, Summer 2011



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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The **JOSH GOODMAN** group has continued to investigate organic reaction mechanisms using a variety of time-resolved techniques such as pico- and nanosecond absorption spectroscopy and photoacoustic calorimetry. In particular, we 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. We have focused primarily on dissociative return electron transfer (DRET) reactions that involve cleavage of C-C, Si-Si and Ge-Ge bonds.



Memorial Art Gallery

Patrick L. Holland

Associate 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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PATRICK HOLLAND and his research group continue to have fun with research on iron- and cobalt-containing compounds for catalysis. In an NSF-funded project on high-valent iron complexes with metal-ligand multiple bonds, our fundamental studies on three-coordinate complexes with Fe=N bonds led to three more papers from Ryan Cowley that appeared this past year. Sarina Bellows also succeeded in making a new supporting ligand that will lead to the next chapter in this effort! In a DOE-funded project on cobalt catalysis, Tom Dugan discovered an intriguing low-coordinate cobalt system that will soon appear in *J. Am. Chem. Soc.* Catalysis by the cobalt complexes has been the purview of postdoc Aydin Kavara, new graduate student Chi Chen, and undergraduate student Jonathan Goldberg.

This grant also paid for a new X-band EPR spectrometer, which arrived in September. In an NIH-funded project on nitrogen reduction, Meghan Rodriguez discovered an iron system that is capable of breaking the N-N bond of N₂ and producing ammonia, the first time this has been done with iron in well-characterized complexes. In parallel, Karen Chiang completed the characterization of new iron complexes with hydride and thiolate ligands that help to understand nitrogenase.

In a collaborative project with the Eisenberg group, postdoc Bill McNamara and graduate students Matt McLaughlin and Zhiji Han each discovered a new photocatalytic H₂ production system. Matt's paper recently appeared in *Chemical Communi-*



cations, and Bill's and Zhiji's papers are expected to come out soon. This project is starting to incorporate biomolecules and nanoparticles from the Bren and Krauss groups, and we enjoy these collaborations within the department.

This year also saw a "labor of love" come to fruition, the publication of a chapter of *Inorganic Syntheses* devoted to diketiminate complexes. This chapter was co-edited by Pat together with Tim Warren (Georgetown) and Dan Mindiola (Indiana), and featured the work of many group members.

We welcomed a number of new researchers this past year. Postdoc P. M. Gurubasavaraj is our new Guru of synthetic chemistry. We were also joined by new graduate students Wenwen Yao and Chi Chen. Wenwen is expanding our N_2 reduction effort. Chi is a joint student with Dan Weix as co-advisor, and will develop practical organic transformations from our new cobalt catalysts. We also have had a number of summer visitors: Monica Boshart from Whitman College has been with us in the summers of 2010-2011, and **PROFESSOR BRIAN EDELBACH (PH.D. '99)** from Monroe Community College did research in our lab with two undergraduates these summers. Finally, we were happy to have **BEN DIBLE (POSTDOC '06-09)** back with us briefly to finish up a paper on palladium-carbene chemistry.

A number of group members were formally recognized for their achievements. These included Tom Dugan (Weissberger Memorial Fellowship), Karen Chiang (DeRight Fellowship), Ryan Cowley (Hooker Fellowship), Meghan Rodriguez (Latimore Fellowship), and Zhiji Han (Sherman-Clarke Fellowship). Meghan and Karen also received Travel Awards to attend national ACS meetings. Ryan was chosen as the Chair for the internationally attended Gordon Research Seminar on

Inorganic Chemistry that will be held in the summer of 2012. Ryan distinguished himself with a presentation in the 2010 Gordon Research Seminar, and Ryan and Karen stood out in the Gordon Conference with a special joke presentation at the end of the conference! Last but not least, Pat was proud of the group when they stepped up as a team (in his absence) to make a departmental presentation on techniques for safely disposing of spontaneously flammable compounds.

Pat has also had a successful year, with thirteen invited talks at universities and conferences. He wrote invited reviews that were published in *Dalton Transactions*, in *Angewandte Chemie*, in *Nature Chemistry*, and in a book on Nitrogen Fixation. The highlight of Pat's year was a five-month sabbatical at the University of North Carolina at Chapel Hill, where he learned about electrochemistry and electrocatalysis. This travel limited his teaching to courses on Group Theory and Inorganic Spectroscopy, which he enjoyed as always. This year, Pat was also recognized with a Volunteerism Award from the Rochester Section of the ACS in recognition of his work with the Harrison Howe Award, and received a Fulbright Scholar Award that will support a four-month trip to Germany in 2012.

In alumni news, **SALLY ROCKS (PH.D. '09)** moved to a position at FLSmidth, a mining company. **KEYING DING (PH.D. '09)** moved to a postdoctoral position with Bill Tolman and Marc Hillmyer at the University of Minnesota. **SALVADOR PEÑA (B.S. '08)** was admitted to the MD/PhD program at Rochester. **AMANDA MACK (B.S. '08)** moved to a teaching position at Phillips Andover Academy. **JEREMY SMITH (POSTDOC '00-03)** published a groundbreaking paper on a stable iron(V) nitrido complex in *Science*.

Tube Sealing in the lab



William D. Jones

Charles F. Houghton Professor of Chemistry

Ph.D. 1979, California Institute of Technology



RESEARCH INTERESTS

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

CONTACT

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The **JONES** group continues to actively pursue organometallic chemistry and catalysis. We had one new graduate student join the group this year, and two students graduated last fall. Dr. Sabuj Kundu has departed for a postdoc with Maurice Brookhart at UNC-CH, and we have a new postdoc arriving this fall, Dr. Valentin Poirier from the University of Rennes. The lab is at full capacity with 11 people this summer. We are (still) planning renovations for this fall that will expand the capacity to 13 people. 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. These projects have involved a variety of fundamental studies of model reactions, as well as actual catalysis. We have established an important understanding on the factors that control metal-

carbon bond strengths that allows us to make predictions about stabilities. 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 an eighth year, where he handled close to 500 manuscripts last year. He lectured in/at Oviedo, Taiwan, Boston, Durham, Beijing, Lanzhou, Lyon, Hawaii, Chicago, Buffalo, Columbia U., Anaheim, Carleton College, Morocco, Montreal, and France. Two graduate students completed their degrees, **TING LI (PH.D. '10)**, and **MATT GROCHOWSKI (PH.D. '10)**. Ting is now with DuPont in Shanghai, and Matt is doing a postdoc at Penn. St. with Ayusman Sen. Bill

Bill Jones in Errachidia, Morocco



was also elected a Fellow of the American Chemical Society in 2010.

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. This selective feature was also surprisingly seen in the activation of 1-chloroalkanes and 1-cyanoalkanes. Investigations of competitions between various nitriles show a preference based on chain length, consistent with the notion that the metal binds to the chain and then 'walks' down to the end before inserting. With chloroalkanes, the opposite is seen, i.e., all chain lengths compete 1:1. This led to the postulate that binding to the chlorine was rate determining, not the binding to the alkyl chain. Using kinetic techniques, it was determined that a rhodium-methyl bond is 3 kcal/mol stronger than a rhodium-cyanomethyl bond, yet C-H activation adducts of the latter are more stable because reductive elimination leads to the formation of a weaker C-H bond. This analysis is being applied to other substrates to come up with a global understanding of C-H activation thermodynamics and metal-carbon bond strengths.

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, coordination 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 also 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 the meeting of the State Key Laboratory of Elemento-Organic Chemistry in Tianjin. He will also speak at the ISHHC in Berlin and at the Spanish Meeting of Organometallic Chemistry in Castellon. He is also a member of the International Scientific Committee for the International Conference on Organometallic Chemistry 2012. 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.

Andrew S. Kende

Charles F. Houghton Professor Emeritus of Chemistry

Ph.D. 1957, Harvard University



RESEARCH INTERESTS

Total synthesis of alkaloids, terpenes, and antibiotics; rearrangement reactions; synthesis of antineoplastic natural products; chemistry of small rings; chemical and biochemical studies of polyhalogenated xenobiotics and of bacterial autoinducers.

CONTACT

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PROFESSOR KENDE and his wife, Frances continue to enjoy their life in retirement in sunny and hot Scottsdale, Arizona. Professor Kende remains active on the Board of Directors of Organic Reactions, Inc., and participated in the Board meeting at the Denver American Chemical Society Meeting that was on August 28-29, 2011. Future plans include occasional consulting, and a return visit to his scientific colleagues in France sometime in the late Fall.





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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The **KRAUSS** group said goodbye this year to one of its more colorful members. Congratulations to our “old smuggler” **CHRISTOPHER EVANS (PH.D. '11)**, who successfully defended his thesis in April of 2011. Chris has just begun his postdoctoral research fellow position at Northwestern University teaching the physicists there the proper way to make semiconductor quantum dots. Amanda Preske is taking over the synthesis of small molecular clusters of PbSe and PbS and will be studying their aggregation kinetics as a method to understand how the larger lead-salt quantum dots grow in solution. Also, last year Jenneke Jalink left the group to return to Israel and pursue a “real” job in industry. We wish her well in her new position!

Dr. Andrea Lee and Wesley Asher, both co-advised by Prof. Kara Bren, have just completed taking a truly inspirational data

set on the structure and dynamics of hundreds of single Cytochrome c proteins measured one molecule at a time. They have two manuscripts in the works on these findings and we are all anxious to see how they are received, since they imply single molecule methods may be absolutely necessary to capture the richness of protein structure heterogeneity as it unfolds. This past fall Andrea and Wes were also joined on the project by Shaun Shahan (another Bren co-advisee), who is going to try his hand at protein synthesis and expression. Julie Smyder is finishing up an important study on the differences in photophysical properties for CdSe quantum dots when excited with pulsed or continuous wave lasers. This work will hopefully help us to understand important and unresolved discrepancies in the literature on these important materials. Jack Calcines is pushing out final thesis chapters on the role of secondary phosphines in the growth properties of semiconductor quantum rods.





Goergen Hall

Helen Wei used new chemistry discovered in the last two years in the group to become the first person to make a CdS quantum dot with a surface composition that is continuously tunable from all Cd to all S. Unexpectedly, when she makes a completely sulfur terminated quantum dot, the particle stops emitting light! This is an important finding with many potential applications and she will be submitting her first paper on this topic shortly. Dr. Michael Odoi is a new postdoctoral fellow who came last fall and has set up a brand new instrument: an atomic force microscope coupled to an inverted optical microscope. This new “toy” will be used to measure the charge state of individual molecules while simultaneously recording their fluorescence properties.

Working with the groups of Pat Holland and Rich Eisenberg, Fen Qiu explored the use of CdSe quantum dots as photo-sensitizers for the production of hydrogen fuel using sunlight. Fen and co-workers recently had a tremendous breakthrough, as they were able to produce hydrogen for orders of magnitude longer than traditional organic dye photosensitizers. Brad Loesch is using ultrafast optical spectroscopy to explore the process of generating more than one electron per absorbed photon in carbon nanotubes. Finally, sticking with the energy theme, newcomers Greg Pilgrim and Dr. Anni Siitonen have taken up the project of fabricating vertically aligned carbon nanotubes and placing them into a thin polymer membrane for the production of hydrogen from solar energy. Together all their work may someday lead to the fabrication of inexpensive solar cells or cars that could run on hydrogen produced from seawater!

Nicole Briglio is working with peptides from Brad Nilsson’s laboratory and using them to solubilize and sort carbon nanotubes by structure. The unique feature of her experiment is that

the peptides are non-natural and she has in the past two years discovered some really unexpected relationships between the structure of the peptide and the interaction with the nanotubes. A paper on her findings is being written and should be submitted in a month or so. Kelly Sowers is working on a really crazy idea: to use layers of quantum dots as a substrate to stimulate neuron growth with the goal to understand HIV induced neurodegenerative disorder. Lenore Kubie is another Krauss-Bren student who is interested in the photoinduced charge transport between heme containing proteins and carbon nanotubes. Lenore is spending the summer as an intern at the National Renewable Energy Laboratory learning about solar cells firsthand! Cunming Liu is our first and only materials science student who has been very busy studying the excited state dynamics of semiconductor quantum dots.

During the summer the group hosted Victoria Zapata from the University of Rochester and Shanna Smith from Mercer University, who both immersed themselves in their research and the Krauss group summer culture, including attending a Red Wings game!

Finally, Todd is going to try his hand at starting another company this year. He received funding from the University of Rochester’s Technology Development Fund to study the thousand-fold scale up of high-quality quantum dot syntheses to the gram scale or larger, which will form the basis of a company to be incorporated this winter. He is joined in this venture by former University of Rochester student Chris Evans, who is excited about putting his synthesis ideas to practical use.

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

kreilick@chem.rochester.edu

ROBERT KREILICK is enjoying his fourth year as Professor Emeritus of Chemistry. Professor Kreilick's research involves 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. Three years ago, new software was written for the ESR spectrometer and low temperature equipment was brought back into working order. We now have an ESR center which is being used by other chemistry faculty members.



Finger Lakes View

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 had the pleasure of presenting a lecture in the Frontiers in Nucleic Acids Symposium held at the Southwest and Southeast Regional ACS meeting in New Orleans Dec 1 -4, 2010. The symposium was organized by three of Tom's former postdocs, Dick Sheardy, David Graves, and Steve Winkle, along with Jeff Petty. Brent Znosko also was an invited speaker. Brent was a graduate student with Doug Turner with whom Tom had the pleasure of collaborating on NMR structural studies of RNA duplexes. It was great fun to catch up with good friends, especially with the French Quarter only a few blocks from

the hotel. Our 2011 NSF funded Research Experience for Undergraduates program had a total of 31 participants, a record number.



David W. McCamant

Assistant 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 **MCCAMANT** group is doing well, evolving according to the time evolution operator. (Yes, that was a quantum mechanics joke.) We were all excited when Randy Sabatini, working in our lab on solar hydrogen production in collaboration with Rich Eisenberg, received an NSF Graduate Research Fellowship this year. UR Chemistry alum **RANDY MEHLENBACHER (B.S. '10)**, now at Wisconsin, also received an NSF GRFP. Way to go Randies! Randy (Sabatini) completed an interesting study of the inter-system crossing rates in a series of halogenated Bodipy compounds that was recently published in the *Journal of Physical Chemistry Letters*. Kristina Wilson and Barbara Dunlap have been continuing challenging work on two-dimensional Raman spectroscopy. Kristina's work probing the ultrafast dynamics of platinum chromophores designed and assembled by the Eisen-

berg group came together into a very nice *JACS* publication. Justin Rhinehart is continuing to tackle the challenging and oft contradictory spectroscopy of charge-transfer compounds. In the fall, we were joined by a talented new first-year graduate student, Joohyun Lee, who has been put to work building our new picosecond laser apparatus. Postdoc J. Reddy Challa has been continuing to pursue interesting new experiments probing the ultrafast dynamics of nucleic acid monomers and oligomers. Last but not least, Dave has been traveling a lot spreading the word about the value and pain of femtosecond stimulated Raman spectroscopy and correcting a bit of math on the way.

Memorial Art Gallery



John S. Muentner

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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2011 has been a busy year for a retired Chemistry Prof, with more attention paid to his new grandson than to molecular spectroscopy. Spectroscopy is still being done, as evidenced by the paper in the publications section. This publication is one more in the long collaboration with Mark Marshall of Amherst College.

Significantly, this is the first in that collaboration where the experiment was done at Amherst rather than Rochester. I've also begun a new collaboration with Bob Field at MIT and am spending a week every couple of months working with Bob's graduate students.



John with grandson, Corey Edwards at nine months

Bradley L. Nilsson

Assistant 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 **NILSSON** group has had an eventful year. Our research in the area of amyloid self-assembly has continued to progress and we have published a number of articles detailing the role of hydrophobic/aromatic effects on amyloid formation (*Molecular BioSystems*, 2011, 7, 486–496; *Molecular BioSystems*, 2011, 7, 497–510; *Biomacromolecules*, 2011, 12, 2735–2745). We have also reported our discoveries in the area of self-assembling hydrogelators (*Chemical Communications*, 2011, 47, 475–477; *Langmuir*, 2011, 27, 4029–4039). This work has been focused on the analysis of N-functionalized phenylalanine derivatives that self-assemble into amyloid-like structures in water; these amyloid structures induce hydrogelation. We are beginning to explore application of these materials as scaffolds for tissue en-

gineering. In addition to this work, we have made progress in the study of semen-derived amyloid that influences HIV infectivity; this work has been carried out collaboratively with Stephen Dewhurst (Immunology and Microbiology, University of Rochester Medical Center) (*Journal of Biological Chemistry*, 2010, 285, 35488–35496; *Biophysical Journal*, 2011, 100, 1325–1334). This work has identified materials and strategies for the development of anti-HIV microbicides. Our research efforts have been communicated in research talks in a number of venues. Brad has traveled extensively in the last year, including to the International AIDS Society 2011 conference (Rome, Italy; July 2011) and the American Peptide Symposium (San Diego, CA; June 2011). Charles Bowerman, Todd Doran, and John

DiMaio presented posters at the American Peptide Symposium in San Diego. Todd won recognition for his poster and was also invited to give a rapid-fire young investigator talk during the conference. Derek was selected to attend the American Chemical Society Division of Organic Chemistry Graduate Research Symposium in July of this year; he was excited to present the results of his graduate research at the prestigious symposium. We are excited about our research progress and look forward to continued productivity and discovery in the coming year.

Several members of the Nilsson group are nearing completion of their Ph.D. studies and have moved/are moving onto the next steps of their careers. **TIMUR SENGUEN (PH.D. '11)** defended his Ph.D. thesis in January 2011, becoming the first Ph.D. from the Nilsson group! Timur is conducting postdoctoral studies at the Boston Biomedical Research Institute. Timur also recently announced his engagement to Kate; they will be married in October of this year and we offer our congratulations and best wishes! Several other members of the Nilsson group will complete their Ph.D. studies in short order. **DEREK RYAN (PH.D. '11)** defended his thesis in August 2011 and then moved to North Carolina to pursue postdoctoral work in the lab of Professor Marcey Waters at the University of North Carolina (UNC). Charlie Bowerman will defend his Ph.D. thesis shortly after Derek (October 2011). Charlie has secured a postdoctoral position with Professor Joseph DeSimone (also at UNC!), who was winner of the 2011 Harrison Howe Award. Todd Doran anticipates defense of his Ph.D. thesis by the end of the year as well and has accepted an offer to conduct postdoctoral research with Professor Tom Kodadek at Scripps Research Institute, Florida. This fantastic group of students has been instrumental in the substantial progress of the Nilsson group research program. Beth Anderson (postdoctoral fellow 2009–2011) has also completed her time in the Nilsson group and has moved across the street to a position in the Department of Dermatology in the University of Rochester Medical Center. I congratulate these

talented individuals on their achievements and am confident of their future success.

In addition to those students that have left/are preparing to leave the Nilsson group, we have a phenomenal group of students who will continue their efforts here in the coming year. Naomi Lee continues to juggle her graduate work with her military obligations and she will finish her Ph.D. work in the coming academic year. John DiMaio and Ria Swanekamp are entering their fourth year and are busily writing manuscripts and finishing ongoing research projects in the areas of peptide self-assembly. **WATHSALA LIYANAGE (M.S. '11)** completed her M.S. studies this summer and advanced to candidacy for her Ph.D. degree. Annada Rajbhandary joined the group this year and has had a strong start on her research project as well. These dedicated and hard-working students are poised to carry forward the momentum of our group's research program.

SAM ANDERSON (B.S. '11) conducted his senior thesis research in the Nilsson lab this past year. Sam conducted research in the area of low molecular weight, self-assembling hydrogels and contributed as a co-author to three publications in peer-reviewed journals. He has started graduate studies in chemistry at the University of North Carolina (there's a strange attraction to UNC for Nilsson lab alumni!). **ALEX FEDERATION (B.S. '11)** also completed his undergraduate studies this spring. Alex contributed to one research publication as a co-author during his time in the Nilsson lab and has now moved to Harvard University to pursue graduate studies in chemical biology. It is noteworthy that Alex was awarded an NSF predoctoral fellowship to support his graduate studies. Rebecca Levin and Emily Hart joined the lab as undergraduate research fellows during the last year and both will conduct their senior thesis research in the lab.

We're excited by the progress made in the Nilsson group in the last year, both personally and in our research efforts. We anticipate another exciting and eventful year.

Nilsson Group, Summer 2011



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

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After moving to Rochester, the **PREZHDO** group has welcomed many new members and collaborations. Two chemistry graduate students Olena Postupna and Julianne Green have started modeling the ultrafast electron transfer dynamics in molecular chromophore assemblies designed by Rich Eisenberg and Dave McCamant. Physics graduate student Amanda Neukirch is collaborating with Todd Krauss's group on the mechanisms of quantum dot synthesis. Postdoc Dr. Heather Jaeger studies excited state properties and dynamics of nanoscale carbon materials. Postdoc Dr. Vitaly Chaban is investigating liquids in confined environments. He is also in charge of the computer cluster supporting the group's research. Dr. Run Long, a visiting scientist

from the University College Dublin, Ireland, investigates photovoltaic materials based on titanium dioxide.

KIRILL IGUMENCHSHEV (PH.D. '11), formerly in Micha Ovchinnikov's group, finished his Ph.D. research in the Prezhdo group and successfully defended in June 2011. Ahmed Mustafa, a visiting scientist from Egypt, is expected to arrive in Rochester shortly.

Among the people who moved to Rochester with the group, chemistry graduate student Tammie Nelson is working on biological applications of nanoscale carbon, while senior scientist Dr. Yuri Pereverzev studies mechanisms of biological catch-binding. In the summer of 2011, Jeremy Smith, a

Speegle-Wilbraham Aquatic Center in the Goergen Athletic Center





Eastman School of Music at night

bright physics undergraduate has joined the group, working with Dr. Heather Jaeger and Amanda Neukirch. Two former advisees of Prof. Prezhdo, Svetlana Kilina and Dmitri Kilin, obtained faculty positions at the Universities of North and South Dakota, respectively.

Several group members spent the summer of 2011 in national labs, gaining valuable research experience in premier scientific environments. Amanda Neukirch was invited to the Lawrence Livermore National Lab in order to implement the computational techniques developed in the Prezhdo group with the LLNL code. Olena Postupna and Tammie Nelson are working with Dr. Sergei Tretiak in the Los Alamos National Lab.

Over the last year, Oleg Prezhdo and his group members presented a couple dozen invited talks, published over 20 papers, including a book chapter and 5 invited reviews and feature articles. The work by Vitaly Chaban was highlighted on page 17 of the June 25, 2011 issue of the “New Scientist” magazine and on multiple web-pages around the world. Another paper from the group was featured in the January 24, 2011 issue of the *Virtual Journal of Nanoscale Science & Technology*. A paper published in the *Journal of Physical Chemistry* last year made a journal cover.

Oleg Prezhdo organized an International Workshop in the Telluride Science Center, and a symposium at the SPIE optical society meeting. He edited a special issue in *Surface Science*, devoted to graphene. His group obtained two new joint grants from NSF on novel photovoltaic materials and from DOE on computational studies of solar water

splitting. The latter grant involves a collaboration of several theory groups in New York state and adjacent area. In 2011, Oleg Prezhdo had the honor to become an Invited Professor at the Université Paris Est, France.

In 2011, Prof. Prezhdo switched from being an Editor of the *Journal of Physical Chemistry*, to become a Senior Editor of the recently created *Journal of Physical Chemistry Letters*. The Letters is a premier branch of *J. Phys. Chem.*, aimed at selecting the most interesting and urgent papers submitted to the journal. Based on its immediacy index, the Letters rank on par with ACS Nano, Small, Annual Reviews of Physical Chemistry, and Progress in Surface Science. The new journal has speeded up the handling and refereeing of submitted manuscripts: the time from submission to web publication is only 40 days, compared to the 70-90 days typical of the majority of journals.

On a personal note, Oleg’s wife Marina has switched from being a research scientist in a biotech company to helping Oleg with the *J. Phys. Chem. Letters*. Marina’s & Oleg’s older daughter Eugenia (20) is a student at the University of Rochester with major in Math and minor in Brain and Cognitive Science. Eugenia’s first paper just got accepted in the *Biophysical Journal*. She spent the summer of 2011 with an REU fellowship in Rice University, applying the two-photon microscopy to studying the brain response to visual stimuli in mice. Their younger daughter Natalie (7) has finished the 1st grade in the Council Rock Elementary in Brighton. She is a regular in the Rochester Chess Club.

Lewis J. Rothberg

Professor of Chemistry

Ph.D. 1983, Harvard University



RESEARCH INTERESTS

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

CONTACT

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LEWIS ROTHBERG'S research group is making progress on many fronts. We are fortunate this year to have obtained another grant from the Department of Energy for plasmonic applications to solid-state lighting technology with Ching Tang and eMagin corporation. Millard Wyman, collaborating with Ulli Scherf from Germany on delayed luminescence in polymers, is progressing rapidly towards graduation along with Steve Paquette who has surprising and exciting results on chromophore stabilization near nanotextured silver. We also expect both Kelly Sassin, who is working on blue phosphor photophysics, and Xiao Wang, who is developing reflective interferometric detection for high throughput analysis of biomolecular binding interactions, to graduate during this coming year. Meanwhile, Chi-Sheng Chang has done great work developing oxide-capped metal nanorods and showing that they have useful and controllable optical properties while being very thermally stable. He is assembling the nanorods into arrays and integrating them with devices in collaboration with Philippe Fauchet's group in engineering. Ben Martin has pulled together a beautiful confocal microscopy apparatus and obtained exciting new results on single conjugated polymer chain luminescence. New graduate students Chris Favaro and Zanny Stwertka are beginning their research, Chris interning with Junji Kido in Japan on organic photovoltaics this summer and Zanny setting out to look at femtosecond transient absorption in conjugated materials. Finally, we are fortunate to have an excellent

new postdoctoral student, Alex Shveyd, who joined us under the auspices of the DOE solid-state lighting program and has quickly applied new analytical methods to understanding chemical degradation in organic LEDs.

Working with undergraduates in the lab and sending them off to outstanding graduate institutions is one of the greatest pleasures of the job and this year the group was delighted to host **DAVID WEINBERG (B.S. '11)** who graduated with high honors and is off to Northwestern. David showed exemplary perseverance, curiosity and creativity in his senior thesis and we wish him the best. This summer we had a very productive REU student, Justin Vadas, working on measuring luminescence quantum yields and a bright high school student, Caity Wischermann, who is studying surface attachment chemistry as relevant to our biomolecular sensing efforts. We are looking forward to continuing our work with undergraduate Jonathan Raybin who will be investigating the photophysics of polythiophenes for his senior thesis.

The intellectual atmosphere in the group is greatly enhanced by a number of dedicated and active senior scientists including William Begley, Al Marchetti, Barbara Stwertka and Ralph Young. Not only do they advance science but they also serve as excellent role models and teachers for both Lewis and the students. We are grateful for their many contributions.

Lewis once again taught the advanced spectroscopy lab (CHM 232) and was grateful for help from Ray Teng and Ben Martin in addition to the teaching fellows. Lewis is beginning to overhaul the course manual to bring it up to date so he can leave this remarkably sophisticated laboratory course built by John Muentner and Bob Kreilick in good shape to be taught by another faculty member. Lewis also returned to teaching second semester general chemistry (CHM132). This year, Lewis participated for the first time in the peer-led team learning (PLTL) training and workshops. The training was both enjoyable and educational for Lewis and, we hope, also improved the educational experience for the teaching fellows and students. Lewis is very grateful to Jim Farrar and Catherine Perez who included him and the TAs in





Wilson Commons

the PLTL workshop classes and mentored Lewis on developing suitable materials for peer learning exercises. It is with considerable sadness that Lewis also thanks Jack Kampmeier for developing the PLTL methodology. Jack died in March and will be greatly missed for his energy and devotion to students, colleagues and the institution. Lewis' father, Abraham, also a dedicated and revered educator and author, died two days after Jack. Lewis would also like to pay respects to an outstanding colleague Prof. Paul Barbara at UT Austin who passed away and to our coworker Jack Fraser, Lewis' primary contact in the technology transfer office. There were, however, also great joys this past year such as visiting the White House to see Lewis' mother Esther Conwell receive the National Medal of Science from President Obama, celebrating our valued colleague Ching Tang's receipt of the Wolf Prize and Rich Eisenberg's induction into the National Academy of Science.

Lewis presented work at a large number of meetings and institutional seminars. This year he was program chair for the Optical Probes of Conjugated Polymers 2011 meeting held in Santa Fe jointly with the Excited State Processes meeting. It is the ninth Optical Probes meeting, the successful series having been started by Lewis and Valy Vardeny in 1991. Lewis and Todd Krauss also had the fun of being on WXXI radio to comment on the NSF-sponsored NOVA series on Materials Science and partici-

pating in a program around that series at the Rochester Museum and Science Center. Along with wife Shelby Nelson, Lewis did hands-on science with inner city middle school students in the Seeds for College program initiated by our colleague in Anthropology, Ayala Emmett.

The company spun off from the work done by Huixiang Li in Lewis' lab nearly 10 years ago, Diffinity Genomics, is progressing. They maintain R&D space rented in Hutchison and manufacture product in Henrietta, now selling pipette-based polymerase chain reaction cleanup kits for over a year. It was extremely gratifying that the product received an award from *The Scientist: Magazine of Life Sciences* in December for being one of the top ten innovations in the Life Sciences in 2010.

Family life continues to be a source of peace and joy. Shelby, Charles (8), and Vivian (7) are all happy and healthy. Shelby's work at Kodak is going extremely well and she seems to find time for a thousand other things too. Charles is in a new school and taking on new experiences like sleepaway camp and playing squash. Vivian starred in her school play and is thriving at a spectrum of activities from horseback riding to gymnastics to art. She entered two pieces in the Rochester modern art museum's 6X6 festival.

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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I began the year in June 2010 with a trip to the Reaction Mechanisms Conference at the University of Massachusetts, followed by a visit to Anne and the two granddaughters in Concord, NH. In August, Anne, the girls, and I visited the Stratford (Ontario) Shakespeare Festival. The high point was a performance of "The Tempest" with the great Christopher Plummer as Prospero. In October I was on a bicycling tour in the Po Valley region of Italy. It is mainly flat, which means less interesting scenery but was good for my aging legs. Afterward I spent three days in Bellagio on Lake Como, which does have spectacular scenery. I had last

seen this area as a young soldier at the end of WW II in 1945. On my return I had a welcome visit from a former grad student, John Borchardt. Anne, the girls, and Claude came to Rochester for Christmas. In May, Anne, the girls, and I went on the Geva London Theatre Tour which included four plays, one of them "As You Like It" at the replica of Shakespeare's Globe Theatre. Finally, my scientific interests continue at a slowing pace. I have lately been doing Gaussian calculations of product proportions in elimination reactions, a topic that my group studied experimentally back in the 1960's.

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 continued research in radiochemistry, heavy-ion reaction dynamics, as well as in technical R&D, but added a new research program in nuclear plasma physics.

Experimental and theoretical results on cluster emission in heavy-ion induced reactions have been presented by several group members at national and international conferences or laboratories. The emphasis in both, the experimental and theoretical work has been to identify dynamic and equilibrium-statistical modes of nuclear fragmentation and cluster emission. Theoretically, present understanding of nuclear instability against boiling and cluster evaporation

has been advanced in an interacting Fermi gas model. This area remains an important research focus by the group. A renewed, generous three-year commitment by the Department of Energy to support the group's heavy-ion research is gratefully acknowledged.

Opening a new research program directed toward nuclear fusion energy production, the group started work on light-ion processes in laser induced thermonuclear plasmas. Corresponding first experiments have been approved by the Basic Science program of the Laboratory for Laser Energetics at the University of Rochester.

Graduate students Mike Quinlan and Iwona Pawelczak presented talks at professional meetings and at several national and foreign nuclear laboratories. Udo was invited to participate at the JINA International Workshop on Nuclear Physics In Hot Dense Matter (London, UK) and the DOE/NNSA Basic Research Directions Workshop on User Science at the National Ignition Facility (Crystal City, D.C.), where he gave a panel presentation.

The Advanced Nuclear Science Education Laboratory (ANSEL) was given for the second time, now oversubscribed by undergraduate and graduate students in Chemistry, Physics and Engineering. Creation of the lab has been funded by a grant from the NRC and continues to be strongly supported by the Chairs of Chemistry and Physics Departments, as well as by the Medical Center and the Laboratory for Laser Energetics.

Research Associate Hardev Singh has returned to a position at the University of Chandigarh/India. Nuclear chemistry graduate student Iwona Pawelczak defended her Ph.D. thesis and has accepted a postdoctoral position at Lawrence Livermore National Laboratory. Mike Quinlan is ready to submit his thesis. Three new graduate students have joined the nuclear chemistry group.

The nuclear chemistry group issues preprints of research papers prior to publication in regular scientific journals. To answer questions, the image included on the lower right corner of the preprint covers (see below) depicts the sculpture “Triad” by the local Scottsville artist Nancy Jurs. It is meant to illustrate the concept of intellectual debate among scientists, which is central to the conduct of science. In a letter to Udo, the artist expressed her delight to permit the use of the image on the group’s preprint covers.



Udo in Berlin, Germany





RESEARCH INTERESTS

Computer modeling of proteins, nucleic acids, and interactions with small molecules; algorithms for molecular dynamics and statistical mechanics simulations.

CONTACT

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HARRY STERN'S graduate student **MIN-SUN PARK (PH.D. '11)** (in the Biophysics, Structural & Computational Biology program) completed his Ph.D. in January 2011 and has started a postdoc in the Gonen Laboratory at the U. Washington Department of Biochemistry and the HHMI Janelia Farm Research Campus. This year, Min-Sun continued his work on molecular dynamics simulations of the G protein $\beta\gamma$ heterodimer, in collaboration with Dr. Alan Smrcka in the UR department of pharmacology. He also worked on treating the problem of variable protonation states and proton uptake/release in protein-ligand binding. Papers describing these projects recently appeared in *Proteins: Structure, Function, Bioinformatics*.

Undergraduate Maruf Sarwar worked on modeling complexes of fumarate reductase, an enzyme that is part of the anaerobic respiratory chain in prokaryotes, to various dicarboxylate ligands. This work was performed in collaboration with Dr. Tina Iverson at Vanderbilt University and was recently published in the *Journal of Biological Chemistry*.

Eva, Danny, and Connor continue to make life interesting for their parents. Eva has just started first grade, accompanied by the required armamentarium of school supplies including two pump bottles of hand sanitizer, a package of dry-erase markers, and twenty glue sticks. She loves animals, reading books to her younger brothers, and eating both kinds of food (orange and white mac & cheese). Danny will be 4 in October and evinces a practical, hands-on approach to life. He has taught his parents many new things: how to throw a lemon so that it hits the kitchen ceiling with maximum velocity, how to strike a beach ball with a broom so that it heads towards Park Avenue with maximum velocity, and how to floor-surf with a baguette.

In what seems like the blink of an eye Connor is no longer a baby but a full-fledged kiddo running around with his brother and sister. He loves being read to, charging headlong fully clothed or not into any body of water from a bathtub to a lake, tackling his brother, trying to chew the tires off of matchbox cars, and climbing in the dishwasher.



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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An exciting aspect of the Rochester environment is that it facilitates a wide range of research because the students and faculty are excellent and collaborative. This year's research reflects those characteristics. Published papers ranged from applications of RNA folding algorithms to fundamental physical chemistry. Walter Moss and Sal Priore published a paper predicting several new RNA structures in influenza virus. Along with Indee Dela-Moss, Tian Jiang and Jayson Baman, they are now experimentally testing these predictions. Jayson is a Rochester undergraduate participating in the summer Research Experience for Undergraduates (REU) program run by Tom Krugh. Much of the bioinformatic approach to influenza RNA follows that developed by Walter when studying a retrotransposon RNA from silk moths in collaboration with Tom Eickbush in the Biology Department. Walter wrote a review including that work and **MICHAEL LOPEZ (B.S. '11)** is a coauthor on that paper. The hope is that studies on influenza RNA will provide insights into development of therapeutics. Toward that end, **RUITING LIANG (PH.D. '10)** along with Ela and Ryszard Kierzek published a paper reporting binding of oligonucleotides on microarrays to an RNA domain from a common catalytic RNA, RNase P. The results were surprising because several oligomers bound to base paired regions, but large regions known not to be paired in the RNase P secondary structure did not bind oligomers. The latter regions are known to form tertiary interactions. The results suggest that microarray binding experiments may sometimes be more efficient than bioinformatics approaches for generating lead oligonucleotide sequences for potential therapeutics.

One of the bioinformatics approaches used for influenza relies on the thermodynamics that the group has developed over many years. **BIAO LIU (PH.D. '10)** used his fluorescence competition assay to improve the model for predicting stabilities of multibranch loops. This was work started by **DAVE MATHEWS (PH.D. '01)** and **JOSH DIAMOND (B.S. '01)**, when they were a graduate student and undergraduate, respectively. It will be interesting to see if the three-

way multibranch loops predicted for influenza support the revised model. Amanda Fisher, an RIT student in our REU program, is now working with Jon Chen and Doug to improve the models for predicting stabilities of internal loops with three mismatches. This is part of a collaboration with **GANG CHEN (PH.D. '05)**, **BRENT ZNOSKO (PH.D. '04)** and **SUSAN SCHROEDER (B.S. '95, PH.D. '02)** to improve parameters for all internal loops.

The group is also laying the foundation for prediction of three dimensional structure. Toward this goal, Scott Kennedy recognized a new 3D motif when comparing an NMR structure determined with **YELENA LERMAN (B.S. '07, M.S. '11)** to structures determined by Gang Chen. The motif contains three sheared purine-purine pairs. Scott and Doug had several discussions about what to name it. In the end, 3RRs was chosen over ArrG. The R and r stand for purine and the motif always contains adenosines (A) and guanosines (G).

To try to understand why RNA forms particular 3D motifs, the group has been working with Harry Stern to improve force fields for predictions, which can then be compared to NMR experiments. **ILYAS YILDIRIM (PHYSICS PH.D. '08)** with help from Scott Kennedy and Jason Tubbs studied the single stranded oligoribonucleotide, GACC, and found that revising parameters for a single dihedral angle, chi, greatly improves predictions of NMR spectral features.

The group's research was recognized by Doug winning the Gordon Hammes Lectureship for 2011. This is funded by the journal, *Biochemistry*, and the Biological Chemistry Division of the ACS. Gordon Hammes is one of Doug's heroes so it was a thrill to win the award. Doug was also moved by the fact that he was originally nominated by former students, **PHIL BEVILACQUA (PH.D. '93)** and **MATT DISNEY (PH.D. '02)**. The lecture was given on August 31st, 2011 at the Denver ACS meeting and followed two hours later with a talk at the University of Colorado, Boulder. Doug slept well that night.



Winter Scene at Mt Hope Cemetery

Biao Liu and Ruiting Liang received their Ph.D.'s. Biao started a postdoc with Matt Disney at Scripps - Florida. Ruiting is a scientist at Avecia Biotechnology in Boston. Michael Lopez received his B.S. and left to pursue a Ph.D. in Chemistry at UCLA, where in addition to his graduate fellowship he was awarded the Eugene V. Cota-Robles Fellowship for his first year. The group welcomed back Ela and Ryszard Kierzek for this summer. Ela and Doug were awarded a collaborative NIH grant, "Folding RNA: Influenza," that will support their collaboration for 3 years.

This year, Doug taught: (1) the lab for first semester General Chemistry, (2) a critical thinking course, "Interface of Chemistry and Biology", that integrated critical thinking of papers with class meetings with seminar speakers, (3) a seminar course for first year graduate students to facilitate their transition to the Department, and (4) a Biophysical Chemistry course. The latter was primarily taught with Dave Mathews and Alan Grossfield, with additional lectures by Clara Kielkopf and Dmitri Ermolenko, all from the Department of Biochemistry and Biophysics. In many ways, Doug was also a student in the Biophysical Chemistry course because he sat in on many of the lectures and essentially all the student presentations. He has always believed that it was best for him to "stay in school."

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 **PROFESSOR DANIEL WEIX'S** group concerns the development of new catalytic methods for the formation of C-C, C-X, and X-X bonds. The group has continued to focus on the direct reductive coupling of two electrophiles, which has rapidly developed into a long-term theme for the group. The reactions are generally operationally simple (tolerant of moisture and air, mix and heat), but present a daunting mechanistic problem. We have reported recently on a new reductive coupling, the reductive conjugate addition of haloalkanes to enones, which 4th year Ph.D. student Ruja Shrestha developed. Daniel Everson (3rd year Ph.D. student) has developed an improved catalyst

system for the cross-coupling of bromoarenes with bromoalkanes, which we will submit for publication shortly. The next 6 months should be busy, with new methods for the synthesis of ketones, Csp³-Csp³ bonds, carbocycles, heterocycles, and diarylmethanes close to fruition. Even more exciting is the progress that postdoctoral researcher Dr. Soumik Biswas has made on understanding the mechanism of the original reductive cross-coupling method. Preliminary results strongly suggest a mechanism that features three different nickel oxidation states and polar as well as radical steps. Finally, this work is now funded by a grant from the National Institutes of Health worth about 1.45 million



Weix group member works in our newest glove box

dollars. We are grateful to the NIH for this new support as well as the University of Rochester and the Petroleum Research Fund earlier support.

Our group has continued to grow with first-year graduate students Lukiana Anka-Lufford, Stephanie Dorn, and Laura Ackerman joining this past year. With new graduate student Chi Chen, we have begun a new collaboration with Professor Patrick Holland on the development of new reactions based upon low-coordinate, high-spin cobalt complexes. Several new undergraduate students have joined the lab: Joeseeph Buonomo ('13), Adam Lee ('12), David George ('13), and Maxwell Hecht ('13). We are also hosting Alexis Kurmis, an I. I. Rabi Scholar from Columbia for the summer. Dan was a Rabi Scholar many years ago. With all the new faces, we have outgrown our space in 421/422 Hutchison Hall and have expanded to 443 Hutchison as well. Finally, our first (under)graduate crossed the stage in May! Congratulations to **BRITTANY JONES (B.S. '11)** and best of luck at USC!



Several group members have been recognized for their efforts in the lab and the classroom this past year as well. Laura Ackerman was awarded a National Science Foundation Graduate Research Fellowship, which provides funding for three years, and a W. D. Walters teaching award. Finally, Ruja Shrestha was selected to attend the 2011 Division of Organic Chemistry Graduate Research Symposium.

Weix Group, Summer 2011



Includes publications accepted or submitted between July 2010 and June 2011.

ROBERT K. BOECKMAN, JR.

Synthetic and Mechanistic Studies of the Aza-Retro-Claisen Rearrangement. A Facile Route to Medium Ring Nitrogen Heterocycles. R. K. Boeckman, Jr., N. E. Genung, K. Chen, and T. R. Ryder, *Org. Lett.* **2010**, *12*, 1628-1631.

Isoamidinium Salts: A New Class of Chiral and Achiral Dienophiles for Diels-Alder Reactions. R. K. Boeckman Jr., Y. Miller, and T. R. Ryder, *Org. Lett.* **2010**, *12*, 4524-4527.

Total Synthesis of a Possible Specific and Effective Acid-targeted Cancer Diagnostic, a Camphor Derived Bis-N-oxide Dimer. R. K. Boeckman Jr., Y. Miller, D. Savage, and J. E. Summerton, *Tetrahedron Lett.* **2011**, *52*, 2243-2245.

KARA L. BREN

A Heme Fusion Tag for Protein Affinity Purification and Quantification. W. B. Asher and K. L. Bren, *Protein Science* **2010**, *19*, 1830-1839.

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Integer Charge Transfer States in Organic Light-emitting Diodes: Optical Detection of Hole Carriers at the Anode Organic Interface. A. P. Marchetti, K. E. Sassin, R. H. Young, L. J. Rothberg, and D. Y. Kondakov, *J. Applied Phys.* **2011**, *109*, 013709-013717.

Kinetics and Mechanism of Single-Stranded DNA Adsorption onto Citrate-Stabilized Gold Nanoparticles in Colloidal Solution. E. M. Nelson and L. J. Rothberg, *Langmuir* **2011**, *27*(5), 1770 - 1777.

Conjugated Polymers: Watching Polymers Dance. L. J. Rothberg, *Nature Chem.* **2011**, *3*(6), 425 - 426

W. UDO SCHRÖDER

N-STAR-A Capture Gated Plastic Neutron Detector, I. A. Pawelczak, J. Tóke and W. U. Schröder, *Nucl. Instr. Methods Phys. Research A.* **2011**, *629*, 230.

HARRY STERN

Benchmarking AMBER Force Fields for RNA: Comparisons to NMR Spectra for Single-stranded r(GACC) are Improved by Revised χ Torsions. I. Yildirim, H. A. Stern, S. D. Kennedy, J. D. Tubbs, and D. H. Turner, *J. Phys. Chem.* **2011**, *115*(29), 9261-9270.

Geometric Restraint Drives On- and Off-pathway Catalysis by the Escherichia coli Menaquinol:Fumarate Reductase. T. M. Tomasiak, T. L. Archuleta, J. Andrell, C. Lunz-Chavez, T. A. Davis, M. Sarwar, A. J. Ham, W. H. McDonald, V. Yankovskaya, H. A. Stern, J. N. Johnston, E. McLashina, G. Cecchini, and T. M. Iverson, *J. Biol. Chem.* **2011**, *286*, 3047.

Conformational Flexibility and Binding Interactions of the G Protein $\beta\gamma$ Heterodimer. M. S. Park, A. V. Smrcka, and H. A. Stern, *Proteins: Struct., Funct., Bioinf.* **2011**, *79*, 518.

Estimating Binding Affinities by Docking/scoring Calculations Using Variable Protonation States. M. S. Park, C. Gao, and H. A. Stern, *Proteins: Struct., Funct., Bioinf.* **2011**, *79*, 304.

DOUGLAS H. TURNER

Comparisons Between Chemical Mapping and Binding to Isoenergetic Oligonucleotide Microarrays Reveal Unexpected Patterns of Binding to the Bacillus subtilis RNase P RNA Specificity Domain. R. Liang, E. Kierzek, R. Kierzek, and D. H. Turner, *Biochemistry* **2010**, *49*, 8155-8168.

Fluorescence Competition and Optical Melting Measurements of RNA Three-Way Multibranch Loops Provide a Revised Model for Thermodynamic Parameters. B. Liu, J. M. Diamond, D. H. Mathews, and D. H. Turner, *Biochemistry*, **2011**, *50*, 640-653.

Identification of Potential Conserved RNA Secondary Structure throughout Influenza A Coding Regions. W. N. Moss, S. F. Priore, and D. H. Turner, *RNA*, **2011**, *17*, 991-1011.

NMR Structure of a 4X4 Nucleotide RNA Internal Loop from an R2 Retrotransposon: Identification of a Three Purine-Purine Sheared Pair Motif and Comparison to MC-SYM Predictions. Y. Lerman, S. D. Kennedy, N. Shankar, M. Parisien, F. Major, and D. H. Turner, *RNA*, **2011**, *17*, 1664-1677.

Benchmarking AMBER Force Fields for RNA: Comparisons to NMR Spectra for Single-stranded r(GACC) are Improved by Revised χ Torsions. I. Yildirim, H. A. Stern, J. D. Tubbs, S. D. Kennedy, and D. H. Turner, *J. Phys. Chem.* **2011**, *115*(29), 9261-9270.

The R2 Retrotransposon RNA Families. W. N. Moss, D. G. Eickbush, M. J. Lopez, T. H. Eickbush, and D. H. Turner, *RNA Bio.* **2011**, *8*(5).

DANIEL J. WEIX

Nickel-Catalyzed, Sodium Iodide-Promoted Reductive Dimerization of Alkyl Halides, Alkyl Pseudohalides, and Allylic Acetates. M. R. Prinsell, D. A. Everson, and D. J. Weix, *Chem. Commun.* **2010**, *46*, 5743-5745.

Reductive Conjugate Addition of Haloalkanes to Enones To Form Silyl Enol Ethers. R. Shrestha, and D. J. Weix, *Org. Lett.* **2011**, *13*, 2766-2769.

Lattimore Hall



Bachelors and Masters Degrees Awarded in Chemistry

2011 BACHELOR OF SCIENCE

Paul Alperin ^{2†}
Samuel Anderson ²
Alexander Federation ^{3†}
Brittany Jones
Caitlyn Rose Kennedy ^{3†}
Michael Lopez
David Weinberg ^{3†}
Mark Werner
Christopher Wong ^{2†}
Jacqueline Zaengle ^{2†*}

2011 BACHELOR OF ARTS

Andrew Adams	Xi Li ^{3†}
Kyle Cron ¹	Katerina Mlejnkova
Amy Donke	Doan Morita
Katherine Garner ^{2**}	Eric Nielsen ²
Andrew Kim ^{3†}	Maruf Sarwar ²
Donghyung Ko	Margaret Stevenson ²
Daniel Lane ^{**}	

2011 MASTER OF SCIENCE

Felipe Angel	Tian Jiang
Nicole Briglio	Yunzhe Jiao
Peter Carlsen	Lenore Kubie
David Condon	Yelena Lerman
Genevieve Criss	Arielle Butts
Barbara Dunlap	Bradford Loesch
David Farkas	Yekaterina Lyubarskaya
Christopher Favaro	Benjamin Martin
John Frost	Sarah Paulson
Wathsala G.H.M. Liyanage	Michael Prinsell
Julianne Green	Randy Sabatini
Zhiji Han	Matthew Sharpe
Yu-Wen Huang	Alexander Sokolsky
Steven Jacob	Kelly Sowers
	Michael St. Phillips

DISTINCTIONS

¹Distinction

²High Distinction

³Highest Distinction

[†]Phi Beta Kappa

*Take 5 Scholar (finishing)

**Take 5 Scholar (beginning)

[†]Kauffman Entrepreneurial Fifth

Year (KEY) Student

Class of 2011 Bachelor's Degree Recipients



Doctoral Degrees Awarded in Chemistry

Sarah E. J. Bowman

Development of Spectroscopic Probes of Second-sphere Interactions in Cytochromes c

Kara L. Bren

Postdoctoral Research Fellow at MIT

Christopher Evans

Insights into Quantum Dot Synthesis: Metal-Metal Bond Formation and Particle Growth

Todd D. Krauss

Postdoctoral Research Fellow at Northwestern University

Meagan Evans

Energetics for C-H and C-CN Bond Activation at Rhodium

William D. Jones

Postdoctoral Research Fellow at the University of Chicago

Gregory Frattini

Chapter I: Studies of the Catalytic Mukaiyama Aldol Reactions of Trimethylsilyloxyfuran, Chapter II: The Synthesis of a Photoaffinity Probe for a Caloric Restriction Mimic

Robert K. Boeckman, Jr.

Postdoctoral Research Fellow at the University of Rochester

Matthew R. Grochowski

Hydrodesulfurization Modeling with Iridium, Rhodium, and Nickel Hydrides

William D. Jones

Postdoctoral Research Fellow at Penn State

Ting Li

Experimental and Theoretical Investigations of C-C, C-H and C-S Bond Activations of Nitriles using Zerovalent Nickel

William D. Jones

Research Scientist at DuPont (China)

Ruiting Liang

Comparison between Isoenergetic Oligonucleotide Microarrays and Chemical Mapping for RNA Secondary Structure Determination

Douglas H. Turner

Analytics Development Chemist at Avecia Biotechnology, Inc.

Biao Liu

Fluorescence Competition Assay Measurements of Thermodynamics for RNA Pseudoknots and Multibranch Loops

Douglas H. Turner

Research Associate at The Scripps Institute – Florida

Iwona A. Pawelczak

Development and Performance Tests of NSTAR, A New Type of Compact Neutron Detector

W. Udo Schröder

Postdoctoral Research Fellow at Lawrence Livermore National Lab

Fehmi Timur Senguen

Clarifying the Determinants of Self-Assembly in the Amyloid- β 16-22 Peptide

Bradley L. Nilsson

Postdoctoral Research Fellow at Boston Biomedical Research Institute

[Strong Auditorium detail](#)



Student Awards

DEPARTMENT AWARDS

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

David Weinberg

John McCreary Memorial Prize

Caitlyn Rose Kennedy

ACS Rochester Section Award

Alexander Federation

ACS Inorganic Chemistry Award

Mark Levin

Merck Index Award

Jacqueline Zaengle

Chemistry Department Award

Paul Alperin

Andrew Kim

Xi Li

Christopher Wong

ENDOWED DEPARTMENT FELLOWSHIPS

Robert and Marian Flaherty DeRight Fellowship

Wesley Asher, Karen Chiang, Pu Luo

Moses Passer Fellowship

Gerald Manbeck

Elon Huntington Hooker Fellowship

Ryan Cowley, Meagan Evans, Tulaza Vaidya

Arnold Weissberger Fellowship

Charles Bowerman, Todd Doran, Tom Dugan, Derek Ryan

Samuel Allen and Ellen Frances Lattimore Fellowship

Jennifer Ciesielski, Meghan Rodriguez, Ruja Shrestha

Agnes M. & George Messersmith Fellowship

Chris Evans

COLLEGE AWARDS

Janet Howell Clark Prize

Caitlyn Rose Kennedy

Catherine Block Memorial Fund Prize

Emily Redman

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

John Frost

TEACHING AWARDS

W. D. Walters Teaching Award

Laura Ackerman, Kyle Biegasiewicz, Benjamin Hmiel, Kimberly Manbeck, Shaun Shahan

Carl A. Whiteman, Jr. Teaching Award

Caitlyn Rose Kennedy

PHI BETA KAPPA

Paul Alperin, Alexander Federation, Caitlyn Rose Kennedy, Andrew Kim, Xi Li, David Weinberg, Christopher Wong, Jacqueline Zaengle



Fellows '10-'11

Elizabeth Anderson

State University of New York at Stony Brook
2002

Soumik Biswas

State University of New Jersey - Rutgers 2010

Vitali Chaban

Kharkiv National University, Ukraine 2009

Jagannadha (Reddy) Challa

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

Benjamin Dible

University of Utah 2006

Yong Du

University of Hong Kong, Hong Kong P.R.
China 2007

Nathan Genung

University of Rochester 2009

P.M. Gurubasavaraj

Georg-August University, Germany 2007

Heather Jaeger

University of Georgia 2010

Ajdin Kavara

Rackham Graduate School, University of
Michigan, Ann Arbor, MI 2010

Sabuj Kundu

Middle East Rutgers, New Jersey; Indian
Institute of Technology, Bombay, India 2009

David Leboeuf

Université Pierre et Marie Curie (UPMC) 2005

Andrea Lee

University of Wisconsin-Madison, Madison, WI
2007

Matthew Liptak

University of Wisconsin-Madison, Madison, WI
2008

Run Long

Shandong University, P.R. China 2008

Theresa McCormick

Queen's University, Kingston, Ontario, Canada
2008

William McNamara

Yale University, New Haven, CT; Lafayette
College, Easton, PA 2010

Marina Naodovic

University of Chicago; University of Novi Sad,
Serbia 2009

Michael Odoi

University of Massachusetts 2010

Linsen Pei

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

Marie-Pierre Santoni

Université de Montréal, Montréal, Canada
2010

Alexander Shveyd

Northwestern University 2011

Anni Siitonen

University of Jyväskylä, Jyväskylä, Finland 2010

Hardey Singh

Panjab University, Chandigarh, India 2008

Francesca Vitali

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

Xiaoyong Wang

University of Arkansas, Fayetteville, AR 2004

Jing Zhang

Nanjing University, P.R. China 2001

Kaidong Zhang

University of Manitoba, Canada; Lanzhou
University, P.R. China 2009

Seminars & Colloquia

JULY 2010

Iwona A. Pawelczak (University of Rochester)
"Development and Performance Tests of NSTAR, A New Type of Compact Neutron Detector," July 30, 2010

AUGUST 2010

Sarah E. J. Bowman (University of Rochester)
"Development of Spectroscopic Probes of Second-sphere Interactions in Cytochromes c," August 3, 2010

Ruiting Liang (University of Rochester)
"Comparison between Isoenergetic Oligonucleotide Microarrays and Chemical Mapping for RNA Secondary Structure Determination," August 11, 2010

SEPTEMBER 2010

Seymour Rothchild Lecture

Professor Peter G. Schultz (The Scripps Research Institute)
"Synthesis at the Interface of Chemistry and Biology," September 29, 2010

Professor Sukwon Hong (University of Florida)
"Exploring New Ligand Designs for Asymmetric Catalysis," September 10, 2010

Professor John Montgomery (University of Michigan)
"Synthetic and Mechanistic Studies of Nickel-Catalyzed Reactions," September 15, 2010

Professor Efrat Lifshitz (Russell Berrie Nanotechnology Institute and Solid State Institute, Israel)
"Multiple excitons in Blinking-free core/alloy-shell colloidal quantum dots," September 15, 2010

Dr. Thomas R. Simpson (AstraZeneca Pharmaceuticals)
"Discovery of AZD2624: A Potent and Selective NK3r Antagonist to Test the NK3 Hypothesis in Schizophrenia," September 17, 2010

Ting Li (University of Rochester)
"Experimental and Theoretical Investigations of C-C, C-H and C-S Bond Activations of Nitriles using Zerovalent Nickel," September 23, 2010

Professor John Berry (University of Wisconsin, Madison)
"Coordination Complexes with Multiple Inorganic Functional Groups," September 27, 2010

OCTOBER 2010

W. Albert Noyes Jr. Memorial Lecture

Professor Joseph R. Lakowicz (University of Maryland School of Medicine)
"Principles of Fluorescence Spectroscopy with Biochemical Examples," October 18, 2010

Professor Joseph R. Lakowicz (University of Maryland School of Medicine)
"Biophysical Applications of Time Resolved Fluorescence and Advanced Fluorescence Methods," October 19, 2010

Professor Joseph R. Lakowicz (University of Maryland School of Medicine)
"Plasmon Controlled Fluorescence: A New Paradigm Using Fluorophore-Metal Interactions," October 20, 2010

Professor Neil Garg (University of California, Los Angeles)
"Complex Molecule Synthesis as a Fuel for Discovery," October 1, 2010

Professor Nicolai Lehnert (University of Michigan)
"The Many Faces of the Coordination Chemistry of Nitric Oxide and its Significance for the Biosynthesis, Sensing and Detoxification of Nitric Oxide in Biological Systems," October 4, 2010

Professor John Peters (Montana State University)
"Insights into the Biosynthesis and Evolution of Complex Iron-Sulfur Cluster Containing Hydrogenases and Nitrogenases," October 6, 2010

Professor David Jonas (University of Colorado at Boulder)
"Hot Carrier Dynamics in Semiconductor Nanocrystals," October 11, 2010

Professor Claudio Margulis (University of Iowa)

"Controlling the outcome of chemical reactions in room temperature ionic liquids," October 25, 2010

Professor Ruben L. Gonzalez, Jr. (Columbia University)

"Translation factor control of ribosome and tRNA dynamics during protein synthesis," October 27, 2010

Professor Vy Dong (University of Toronto)

"Stereoselective Strategies for Activating C-H Bonds, Carbon-dioxide, and Simple Olefins," October 29, 2010

NOVEMBER 2010

Professor Mark Berg (University of South Carolina) *"MUPPETS: Making Kinetics Interesting Again,"* November 1, 2010

Matthew R. Grochowski (University of Rochester) *"Hydrodesulfurization Modeling with Iridium, Rhodium, and Nickel Hydrides,"* November 2, 2010

Professor Massimo Bietti (Università Tor Vergata, Italy) *"Understanding reactivity patterns of alkoxyl radicals,"* November 5, 2010

Magomedov-Shcherbinina Memorial Lecture

Professor Xiaowei Zhuang (Harvard University) *"Breaking the Diffraction Limit: Nanoscopic Imaging of the Living Systems,"* November 9, 2010

Professor Catherine Drennan (Massachusetts Institute of Technology) *"Crystallographic snapshots of metalloenzyme complexes,"* November 15, 2010

Professor Douglas W. Stephan (University of Toronto) *"Frustrated Lewis Pairs: A New Paradigm for the Activation of Small Molecules and Catalysis,"* November 17, 2010

Stanislav Groysman, Ph.D. (Massachusetts Institute of Technology) *"Metal-Oxo Complexes in Pseudotetrahedral Oxygen-Rich Environments of Dioxo,"* November 18, 2010

Biao Liu (University of Rochester) *"Fluorescence Competition Assay Measurements of Thermodynamics for RNA Pseudoknots and Multibranch Loops,"* November 19, 2010

Brian Popp, Ph.D. (Rice University) *"Enzyme-like Reactivity and Selectivity with Dirhodium-Metallopeptide Catalysts,"* November 29, 2010

DECEMBER 2010

Michael Neidig, Ph.D. (Los Alamos National Laboratory) *"Structure-Property Relationships in Transition*

Metal Systems: From Bioinorganic Catalysis to Nanoclusters and Catalytic Materials," December 2, 2010

Amanda J. Morris, Ph.D. (Princeton University) *"Solar Fuel Generation from a Carbon Dioxide Feedstock: A Mechanistic Investigation,"* December 6, 2010

Daniela Buccella, Ph.D. (Columbia University) *"Fluorescent Sensors for Visualizing and Quantifying Mobile Zinc in Biology,"* December 9, 2010

Christopher Scarborough, Ph.D. (University of Wisconsin, Madison) *"Part I. Axially-Chiral Seven-Membered N-Heterocyclic Carbene Ligands Part II. Coordination Chemistry of the Radical Anion of 2,2'-Bipyridine and the Paucity of Intermediate-Spin Chromium(II),"* December 21, 2010

JANUARY 2011

Professor Joseph Grabowski (University of Pittsburgh) *"Assessing Undergraduate Research Programs - Moving Beyond Anecdotes,"* January 21, 2011

Fehmi Timur Senguen (University of Rochester) *"Clarifying the Determinants of Self-Assembly in the Amyloid- β 16-22 Peptide,"* January 24, 2011

FEBRUARY 2011

Hutchison Memorial Lecture

Professor John Hartwig (University of Illinois at Urbana-Champaign) *"The State of Catalyst Design - Cross-Coupling as a Case Study,"* February 21, 2011

Professor John Hartwig (University of Illinois at Urbana-Champaign) *"Catalytic Functionalizations of Alkanes and Arenes,"* February 22, 2011

Professor John Hartwig (University of Illinois at Urbana-Champaign) *"Iridium-Catalyzed Asymmetric Allylic Substitution,"* February 23, 2011

Professor Paul Dunman (University of Rochester School of Medicine and Dentistry) *"MRSA vs MRSA,"* February 2, 2011

Professor Trevor W. Hayton (University of California at Santa Barbara) *"Synthesis and Reactivity of an Electrophilic Uranium Nitride,"* February 7, 2011

William Spencer (University of Rochester) *"The Development of N-Heterocyclic Carbene-Boranes as Tunable*

Radical Reducing Agents, February 11, 2011

Professor Samuel Johnson (University of Windsor) *"The Fast and the Furious: Do Nickel Complexes Activate C-H or C-F Bonds?,"* February 14, 2011

Professor George Schatz (Northwestern University) *"DNA structures, excited states and nanomaterials,"* February 16, 2011

Joshua Brooks (University of Rochester) *"Silyloxy-Based Alkyne Metathesis Catalysts,"* February 18, 2011

MARCH 2011

Dr. Robert Tycko (National Institutes of Health) *"Amyloid Fibril Structure: Insights from Solid State NMR,"* March 2, 2011

Jessica M. Smith (University of Rochester) *"Probing PKS and NRPS Protein-Protein Contacts: Cross-Linking Studies,"* March 4, 2011

Brad Loesch (University of Rochester) *"Ultrafast Relaxation Dynamics in Single Walled Carbon Nanotubes,"* March 14, 2011

Professor Peter Wipf (University of Pittsburgh) *"Total Synthesis of Stemonon and Ergot Alkaloids,"* March 16, 2011

Daniel Everson (University of Rochester) *"Cyclopropenium Ion: New Twists on Old Chemistry,"* March 18, 2011

John DiMaio (University of Rochester) *"Peptoids as Biological Tools,"* March 25, 2011

APRIL 2011

Victor J. Chambers Memorial Lecture

Professor Andrew Myers (Harvard University) *"Evolution of a Practical Synthetic Route to the Tetracycline,"* April 18, 2011

Professor Andrew Myers (Harvard University) *"Antiproliferative Natural Products with Promise in Cancer Research,"* April 19, 2011

Professor Andrew Myers (Harvard University) *"Antiproliferative Natural Products, Synthesis and Mechanistic Study,"* April 20, 2011

Ria Swanekamp (University of Rochester) *"Endoperoxides as Anti Malaria Agents,"* April 1, 2011

Meagan Evans (University of Rochester) *"Energetics for C-H and C-CN Bond Activation at Rhodium,"* April 1, 2011

Eric Henry (University of Rochester) *"Isotopic Effects in Nuclear Transmutation and Decay: The Reactions $78,86\text{Kr} + 40,48\text{Ca}$ at $E/A = 10\text{MeV}$,"* April 4, 2011

Professor Elizabeth Jarvo (University of California, Irvine) *"Mechanism-Based Design and Development of Catalytic Reactions,"* April 8, 2011

Professor Frank V. Bright (State University of New York, Buffalo) *"Trekking Toward Nanoscale Sensors,"* April 11, 2011

Professor Ronald T. Raines (University of Wisconsin, Madison) *"Electronic Effects on Protein Structure,"* April 13, 2011

Michael Prinsell (University of Rochester) *"Double C-H Activation,"* April 15, 2011

Gregory Frattini (University of Rochester) *"Chapter I: Studies of the Catalytic Mukaiyama Aldol Reactions of Trimethylsilyloxyfuran, Chapter II: The Synthesis of a Photoaffinity Probe for a Caloric Restriction Mimic,"* April 15, 2011



Christopher Evans (University of Rochester)
"Insights into Quantum Dot Synthesis: Metal-Metal Bond Formation and Particle Growth," April 15, 2011

XiaoJu Zhang (University of Rochester) *"The MD Simulation Study of tRNA Modifications,"* April 21, 2011

Salvatore Priore (University of Rochester)
"RNA Structure Discovery in Influenza A Virus," April 21, 2011

Professor Roger Loring (Cornell University)
"Dielectric Noise and Noncontact Friction: Several Adventures of Two UR Alumni," April 25, 2011

Professor Joseph M. DeSimone (University of North Carolina at Chapel Hill) *"Bridging Fields and Harnessing Diversity for the Sake of Innovation,"* April 30, 2011

Harrison Howe Award Lecture

Professor Joseph M. DeSimone (University of North Carolina at Chapel Hill) *"Co-opting Moore's Law: Medicines and Vaccines from a Wafer,"* April 29, 2011

MAY 2011

Sarina Bellows (University of Rochester)
"Properties of Diruthenium Paddlewheel Complexes and Their Applications Towards Molecular Wires," May 19, 2011

Fen Qiu (University of Rochester) *"Water-soluble Quantum Dots for Hydrogen Production,"* May 24, 2011

Biological Chemistry Cluster Seminar

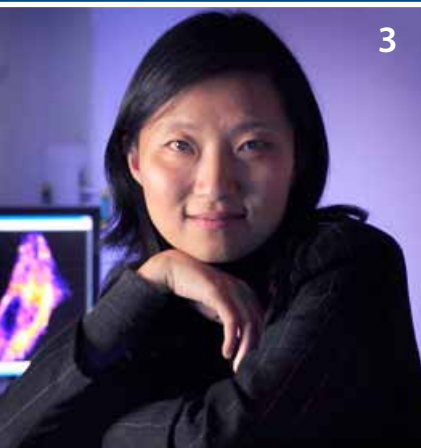
Elizabeth Theil Ph.D. (Children's Hospital Oakland Research Institute) *"Ferritin Protein Nanocages- How Iron moves In, Out & Controls Biosynthesis,"* June 9, 2011

Professor Sachdev Sidhu (University of Toronto, Canada) *"Synthetic Proteins: New Tools for New Biology,"* June 9, 2011

JUNE 2011

Kirill Igumenshchev (University of Rochester)
"Quantum Breathers in Dynamics of a Coherent State," June 3, 2011

Distinguished & Special Lectures



¹ **Peter G. Schultz** Seymour Rothchild Lecture (September 2010)

² **Joseph R. Lakowicz** W. Albert Noyes Jr. Memorial Lecture (October 2010)

³ **Xaiowei Zhuang** Magomedov-Shcherbinina Memorial Lecture (November 2010)

⁴ **John Hartwig** Hutchison Memorial Lecture (February 2011)

⁵ **Andrew Myers** Victor J. Chambers Memorial Lecture (April 2011)

⁶ **Joseph DeSimone** Harrison Howe Lecture (April 2011)

NEWS FROM THE ADMINISTRATIVE STAFF:



KAREN DEAN celebrates the completion of her sixth year in the chemistry department and her 23rd year with the University. As administrative assistant to the chair, the central focus of Karen's efforts are the supervision of staff, administrator of faculty recruiting, administrator of postdoctoral hiring, and the liaison for the chair with the University Deans/Administrators

and the International Services Department. In August of 2011, Karen passed the baton on to her successor, Barbara Snaith, when Karen retired from the University. Her future plans entail some travel, volunteer work within her community and being a full-time mother to her labrador retrievers.

BARBARA SNAITH comes to us from the Department of Orthopaedics and Rehabilitation at the Medical Center. In April 2011, Barbara was the recipient of the 2011 University Staff Community Service Award for her 20 years of volunteering in the Rochester, NY and New York City/Long Island areas. The department welcomes Barb and looks forward to a cohesive working relationship.



DONNA J. DOLAN is a long time staff member in the Department of Chemistry. She is currently beginning her twenty-fourth year in chemistry, now serving as departmental receptionist. In this role, Donna continues to provide support for purchasing in the Chemistry Business Office, and organizes the departmental distinguished speakers program, while providing assistance to faculty and managing the chemistry department's main office. She is now a very proud grandmother for the first time, blessed with grandson Austin James. Proud parents are her son Adam Dolan and new wife Amanda.

KENNETH SIMOLO (PH.D. '85) celebrates his twenty-fourth 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's big project this summer was the new chemistry lab.

LORY HEDGES continues in the development administrator & alumni relations position, having accomplished Clasp Certification in the fall, submitting almost 50 grant applications during the year, updating the department website and learning her way around the University. She has enjoyed planning and executing several events for the department, including the Meliora Weekend Open House, Gates Happy Hour, Magomedov Memorial Lecture, Harrison Howe Award and RichFest. It was much harder to plan the Memorial Service for Jack Kampmeier, who was so helpful during her first year in the department. She is grateful for all the assistance in the department and the great students she has; Breanna Eng and Amanda Chang. She is also the new editor



Donna Dolan and grandson, Austin



on the department newsletter (yes, this!) and has enjoyed the project and learning the software. Many thanks to John Bertola who tutored Lory in the Adobe InDesign software. John remains a wonderful resource to the chemistry department.

TERRI CLARK, now in her fourth year as undergraduate studies program coordinator and course administrator, is celebrating the arrival of her first grandchild, born to youngest daughter, Rebecca, and son-in-law Andrew Wright. Terri and her husband, Ben, traveled to the tri-cities in the state of Washington to greet Del and spend time with the proud parents. While there, they visited their older daughter, Sarah, who will be performing in "The Wedding Singer" (community theatre) this November. Youngest son, Andrew, has moved from California to Oregon to complete his degree at Eastern Oregon University and is now only two hours driving from his sisters in Washington. Still having oldest son Joe and his wife Kristy in California, as well as parents, means time is split up and down the west coast.

ROBIN COOLEY, our graduate studies coordinator, has now been with the department for seven 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 pizza bowling party 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 newest graduate students informed and ready for the start of the new school year. For the 2011-2012 school year, we are welcoming seventeen new graduate students to the department.



LYNDA MCGARRY (M.S. '85) is a new member of the department, starting a position in September 2010 as the administrative assistant to the chair of the materials science program, Professor Todd Krauss. Lynda has been coordinating the graduate student admissions and other committees for the interdisciplinary materials science program, which welcomes five doctoral students and twelve masters

degree students this fall. She was also involved in planning the successful "Nanosymposium 2011 - Applications in Biomedicine" that was held on May 23, 2011 in Goergen Hall.

Lynda also works part-time as an editorial assistant in both the *JACS* and the *JOC* offices, and is very grateful to Valerie Fitzhugh and Terrell Samoriski and all of the people in the department who have been helping her navigate the university procedures. Lynda obtained a B.S. in Chemistry from St. John Fisher College and then earned an M.S. in Chemistry at the UR under the direction of Bill Jones before joining the Eastman Kodak Research Laboratories as a research and development chemist for several years. Lynda was the program manager for the commercialization and scale-up of several new photographic and OLED materials. After leaving Kodak, Lynda obtained an M.S. in education from SUNY Brockport, and received NYS teaching certifications in chemistry and general science. Lynda lives in Spencerport with her husband Dan, her children Claire and Ian, and a schnoodle.



MARGUERITE WESTON,

assistant to faculty, has been with the Department of Chemistry for sixteen years. She coordinates the chemistry seminar program by scheduling rooms, contacting the 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. The most recent proposal was recently submitted in summer 2011. This program attracts approximately 125 applications each year from undergraduates across the nation and the University of Rochester. Marguerite and her husband, Art, are residents of Henrietta, NY and enjoy dancing and gardening.

ELLY YORK, who joined the chemistry department in November of 2006, works as a teaching assistant in the undergraduate laboratories and is the sole TA for the summer sessions of the general chemistry laboratory. Elly also assists with safety inspections in the department, as well as working part-time in the chemistry stockroom. Elly is a graduate of Alfred University and has clinical work experience, having previously worked in several veterinary clinics prior to coming to UR. She also has a Master's degree in education. On July 8th, Elly and husband, Brandon, had their first child, a son named Aaron Timothy. Congratulations!

NEWS FROM THE EDITORIAL OFFICES

KIRSTIN CAMPBELL, coordinating editor, oversees the staff of *Inorganic Chemistry*. Out of 44 journals in their category, *Inorganic Chemistry* is once again the most-cited journal in inorganic chemistry. The Rochester office, the main office of the journal, overseen by Editor-in-Chief Richard Eisenberg, handled over 2,565 manuscripts in 2010. *Inorganic Chemistry* is one of the few ACS journals featuring issues with a changing cover, being published twice a month. *Inorganic Chemistry* is kicking off the 50-year celebration of the journal in 2011 complete with symposia and celebratory events. On a personal note, Kirstin has been busy at home, enjoying and working with her horses. Kirstin has begun riding competitively again, after many years off and has been enjoying a very successful year at local open and county fair shows, hunter paces, horse trials and other events. She recently competed in the Genesee Valley Riding and Driving Club Horse trials and brought home a 7th place in her division.

ARLENE BRISTOL continues to enjoy working part-time as senior editorial Assistant. She excels at her hobby of playing duplicate bridge in her spare time. **MARCIA EISENBERG** continues working part-time, assisting us with travel and serves as an administrative assistant to our growing journal office.

VALERIE FITZHUGH is currently celebrating her tenth year as an editorial assistant in the Department of Chemistry. She served on the journal staff of the *Inorganic Chemistry* EIC office and the *Journal of Organic Chemistry* before assuming her current position as editorial assistant to Associate Editor William D. Jones for the *Journal of the American Chemical Society* (JACS) nine years ago. Interacting with authors, reviewers and the American Chemical Society (ACS)

Aaron Timothy York



Production staff in this role has been an enriching experience for Val. She continues to find the fast pace of the *JACS* office engaging and interesting, and the expertise of newer journal assistant **LYNDA MCGARRY** to the *JACS* office immeasurable in expediting the work-flow. The Rochester office of *JACS* is expected to handle in excess of 500 manuscripts this year. The *Journal of the American Chemical Society*, founded in 1879, is the flagship journal of the American Chemical Society and the preeminent journal in the field. This periodical is devoted to the publication of fundamental research papers in all areas of chemistry and publishes approximately 16,000 pages of articles, communications, book reviews, and computer software reviews 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* received 369,164 total citations and an increase in Impact Factor to 9.019, while publishing more articles (3,139) than any other journal in the category as reported in the 2010 Journal Citation Reports® by Thomson Reuters.

TERRELL SAMORISKI completed her sixth year as editorial assistant for *The Journal of Organic Chemistry* (JOC) in August 2010. 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 now has the pleasure of working with new part-time journal assistant **LYNDA MCGARRY (M.S. '85)** whose inorganic breadth of knowledge will be a tremendous resource. The *JOC* publishes original contributions reporting novel, important findings of fundamental research in all branches of the theory and practice of organic chemistry. Due to the increase in submissions and the implementation of the web-based submission procedure, the journal has expanded to include associate editor's offices in Europe and China. In 2010, the Rochester office handled more than 200 manuscripts. The journal publishes both shorter articles (notes) and lengthier ones (articles), and has added synopses and brief communications as publication options for authors. The covers of the journal continue to be a highly desired forum for authors to showcase art relating to their manuscripts.

SCIENTIFIC & TECHNICAL STAFF

TERRY (TED) O'CONNELL started his twenty-ninth year with the chemistry department and enjoys his position as director of technical operations. He is responsible for new equipment installations and any building renovations. This past year, he has been busy training users on the new mass spectrom-

eters that were purchased last year. He also has added a new part-time member to the technical staff, **JALIL SHOJAIE**. Jalil works mornings in the chemistry department and afternoons at the University Laser Laboratory. He has a solid organic chemistry background and assists researchers in structural determination using the departmental instrumentation.

ERIC LOBENSTINE (PH.D. '81), manager for computers and network, had a year filled with the ordinariness of a technical support role: computer upgrades, network problems to fix and servers to maintain. This year has seen two major projects completed by University IT staff. Hutchison now has WiFi access everywhere; Eric is very happy NOT to run new network cables to every new student's desk. Network security has also been significantly enhanced; a perimeter firewall now prevents hackers from gaining easy access to almost all systems in chemistry's network, without significantly changing how we access our own systems. Long term projects involve upgrading our web and email server software, also for security concerns, as well as starting to plan the replacement of all of the computers running the five departmental NMR instruments. On a personal note, it has been delightful to have Brian here in Rochester working on his M.B.A. at the Simon School. Sadly, though, his summer internship with Parker Hannifin Corp. meant that he was unable to join Ethan (now a senior at the U of R), Jeanne and me on a whirlwind tour of the Scottish Highlands in July. Nine days only allows a taste of this wonderful country, full of wonderful vistas, very helpful and charming people, and incredible single malt whiskeys! You can see the three of us at the summit of Ben Lomond, the mountain overlooking Loch Lomond. The approach that we took went practically straight up for the last 300 feet!

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. In 2011, renovations in Hutchison Hall were undertaken: Rooms B29 and B31 were renovated for Professor Neidig, designing and building the vacuum system for the new undergraduate organic laboratory (102) and relocation of Professor Schroeder's labs to 441 and 442. 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 not only as a coach but "making road trips to watch D3 soccer." Crystallographer **BILL BRENNESEL** has been very busy

running the X-ray Crystallographic Facility (single crystal analysis) and the CENTC Elemental Analysis Facility (bulk sample analysis) this year. Since the sample characterization techniques offered by both facilities are important for the publication of new materials, some researchers are finding it useful to request that the same samples be examined by both. In addition to the X-ray structural determinations performed daily, Bill directs a laboratory section for undergraduate course CHM 234, in which students run a "unit cell determination" and check the results against those in the Cambridge Structural Database, two tasks that are common to every X-ray experiment. In the latter half of each spring semester, he teaches graduate course CHM 416, which offers students a marriage of theory and application: each student learns the fundamentals of crystallography, plus performs and presents a full structural determination on an actual research sample. Students that complete the graduate course become officially trained users of the facility and are encouraged to run samples from their own research. Two doors down from the X-ray facility is the elemental analysis facility, where approximately two milligrams of each submitted sample are burned to determine the absolute percentages of carbon, hydrogen, and nitrogen. The instrumentation is especially geared toward correct examination of air-sensitive samples, those that react with the water and/or the oxygen in the air. Such samples are prepared in a dedicated glove-box that is filled with the inert gas argon. When asked why this facility is so successful in running air-sensitive materials, Bill responded, "It's not difficult to work with air-sensitive samples, but it requires a little patience. The analyzer must be calibrated correctly using a reference of known composition, and the argon atmosphere in the glove-box has to be very pure. As long as both conditions are met and verified, research samples can be examined properly." In

Eric Lobenstine in Scotland with son, Ethan and wife, Jeanne





Muses in front of Meliora Hall

Tunnels under the Quad



the first year and a half that the elemental analysis facility has been available, over 500 samples have been examined.

SUE CARDINAL, chemistry librarian from the Carlson Library, reports that we have a new Arleen N. Somerville Director, Zari Kamerei. She was head of the Science Libraries and Chemistry Librarian at University of North Carolina at Chapel Hill and holds a B.S. in physics and an M.L.S. with a specialty in chemical information from Indiana University. Previously she was a chemical information specialist at Petrolite Corporation in St. Louis.

Carlson continues adding online access to older journals including Elsevier's *Journal of Organometallic Chemistry*, and Wiley's *Liebig's Annalen*. We have added Springer Materials, an online version of Landolt-Börnstein as part of a growing electronic reference collection. This summer we've shifted the journals into a tighter configuration so that we can create new study spaces. Sue spends a few hours each week in the graduate student lounge answering science reference questions.

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. She is even more happy that her daughter, Jessica has graduated from St. John Fisher this year. The business office staff consists of four members with valuable experience. **ANNA KUIITEMS** is responsible for reconciling grant ledgers, P-card management and graduate student payroll, and as backup for Randi Shaw. Anna enjoys working with the faculty, staff and students in the chemistry department. At press time, Anna and her family are sending off son, Chris, to Kazakhstan to volunteer in the Peace Corps. **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 26 years now.

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.

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.

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.

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.

Richard Eisenberg

Chemistry Endowment Fund

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

Magomedov-Shcherbinina Memorial Fund

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

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.

I wish to contribute to the following fund:

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