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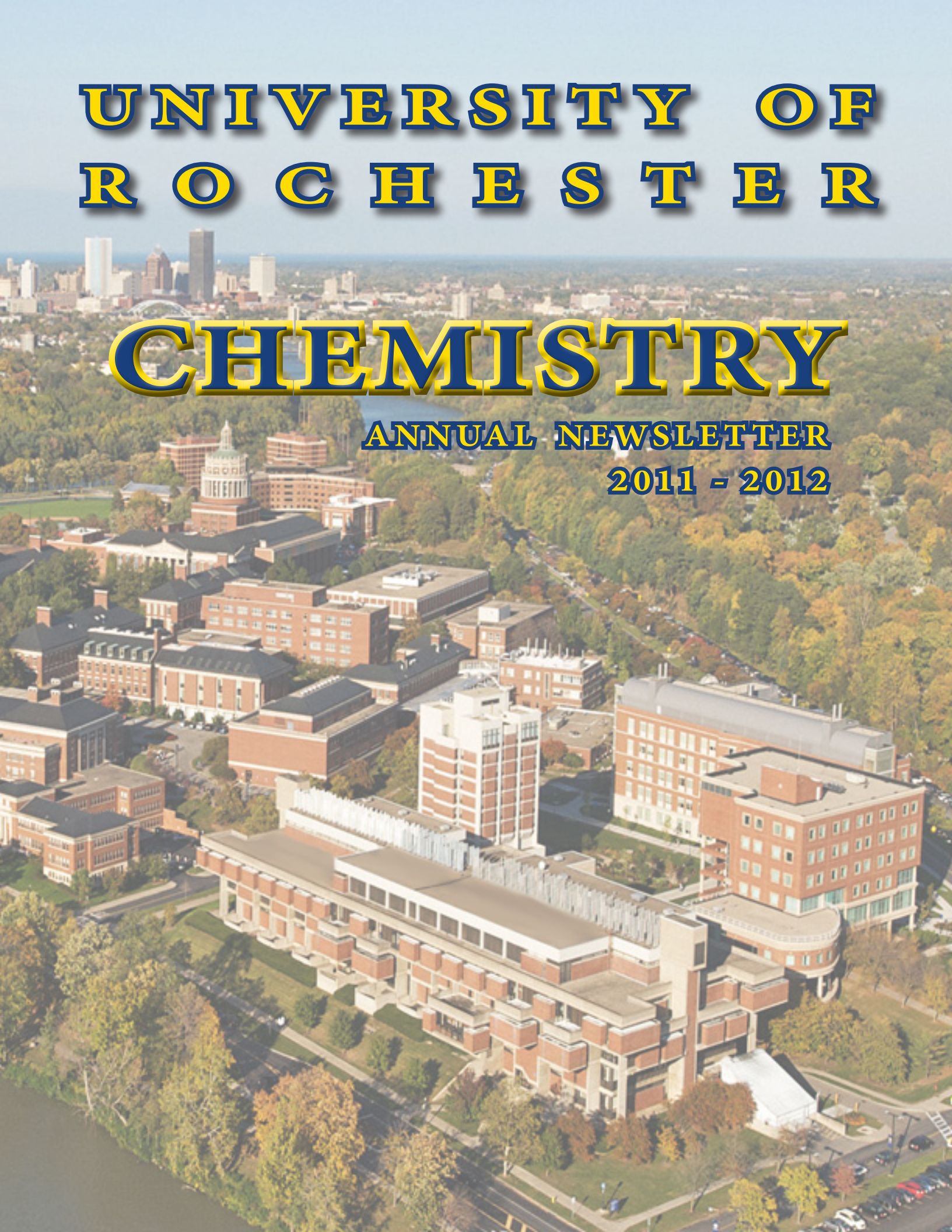

CHEMISTRY

ANNUAL NEWSLETTER
2011 - 2012

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From the Chair

Greetings to all Department of Chemistry Alumni! We enjoyed a busy and productive 2011-2012 year in the department and at the University. As I enter my tenth, and final year as chair of the Department of Chemistry, I am happy to share with you some of the developments within the department and University from the past year.

The economic stress that the US has been experiencing since 2008 continues to have an impact on the University and to 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 endowments. 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 while we have had one faculty departure (Harry Stern moved to a position in the University Research Computing Center), we have hired one tenure-track junior faculty in theoretical chemistry who will join us in July 2013. This past year we added Ben Hafensteiner, a former UR graduate, as an instructor for our large general chemistry and organic laboratory courses. Furthermore, despite an ailing economy, the department has increased sponsored research to $5.5M in 2011 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, NSF, and the Provost's Multidisciplinary Research Award, as well as others. However, given the fiscal stress which the federal government is experiencing and the obvious need to reduce federal deficits, the future 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, 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 who will begin in 2013. Ignacio Franco, will begin next year as an assistant professor of chemistry. Ignacio received his Ph.D. in Theoretical Chemical Physics from the University of Toronto Canada and is currently a Research Group Leader in the Theory Department of the Fritz Haber Institute of the Max Planck Society in Berlin Germany. Ignacio will pursue a research program focused on Molecules under Stress. He will investigate using molecular response to stimuli, such as intense irradiation by powerful lasers, for energy conversion and molecular property manipulation.

Several chemistry faculty received notable awards this year. James Farrar was named a Fellow of the American Association for the Advancement of Science, Patrick Holland spent most of the spring semester in Germany as a Fullbright Scholar, and Douglas H. Turner gave the 2011 ACS Hammes Biochemistry Lecture. These kinds of recognitions help to sustain our efforts to recruit and retain high quality faculty and students, and to 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 three NSF Graduate Research Fellowship Awards and one Honorable Mention. 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 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 serves as a model both for future renovations of our remaining organic laboratories and a basis for planning renovations of our freshman laboratories. The University began a major gift campaign this past fall to help raise funds for these renovations. Through the generous gifts of our alumni and other university and unrestricted funds, we will continue the staged renovation of chemistry's research and teaching laboratories over the next several years.

Our graduate program has experienced sustainable growth with the matriculation of 16 new first year graduate students, bringing our departmental graduate student population to about 120 and our total researchers to over 150. And, for the first time, we approach 50 undergraduate chemistry seniors who will graduate in 2013 with either the Bachelor of Arts or Bachelor of Science Degree.

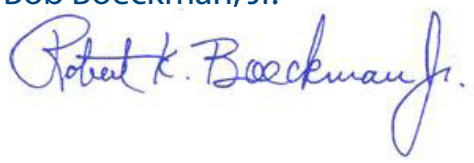
Finally, let me close by thanking all of you for your continuing support of the department over the year. We are fortunate to have the strong support of the College in all our efforts. However, the support and advice of our alumni is an invaluable resource. We are happy to receive news and are proud of your achievements in your respective fields. Please let us know how you are doing by using the reply form at the back of this newsletter or online at http://www.chem.rochester.edu/alumni/submitnews.php. 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 invite you to visit Rochester and attend Meliora Weekend events October 11th – 14th, 2012. 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 at www.chem.rochester.edu. 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.

Meliora and best wishes to all for a successful and happy year in 2012-2013.

Sincerely,

Bob Boeckman, Jr.



The back of Rush Rhees

Donors '11-'12

Includes donations received between July 2011 and June 2012.

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Roger P. Napier (Ph.D. '64)

GIFTS OF $50,000+

Yuh-Geng (M.S. '75, Ph.D. '77) and Margaret H. Tsay

GIFTS OF $10,000+

George G. Stanley (B.S. '75) and Sally Hunter

GIFTS OF $5,000 - $9,999

Bruce D. Roth (Postdoc '82)
Margaret May-Som (M.S. '74, Ph.D. '76) and Wuu-Yong Wu (Ph.D. '74)

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Norman P. (B.A. '52) and Mary G. Neureiter
Thomas J. Perun (Ph.D. '63)
David N. Ridge '74 (M.S.), '76 (Ph.D.)
Joseph P. Smith (B.S. '72)

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Thomas Neil Thompson (B.S. '77, M.S. '81, Ph.D. '85, M.D. '85)

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Alan M. Edelson (B.S. '59)
Thomas A. Henderson (M.S. '83, Ph.D. '86)
John C. Hodges (Postdoc '82 and '83)
Lori C. (B.A. '78) and Richard A. Josephson (B.A. '77)
John Samuel Kruse (B.A. '82, Ph.D. '89, M.D. '90)
Jiong Lan (Postdoc '02)
Norman J. Leister (Ph.D. '58)
Lanny S. (M.S. '74, Ph.D. '77) and Diane Liebeskind
Gordon A. (Postdoc '52) and Mary L. Nicholls
Joseph Weinstock (Ph.D. '52)
Margaret May-Som (M.S. '74, Ph.D. '76) and Wuu-Yong Wu (Ph.D. '74)

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Henry Havel (B.S. '76)
Martin Kunstmann (PH.D. '62)
Roy Alan Leckonby (M.S. '74, Ph.D. '76)
Ronald M. Levinson (B.S. '56)
Frederick Lewis (Ph.D. '68)
William J. Linn (Ph.D. '53)
Margaret Logan (M.S. '72, Ph.D. '82, Postdoc. '88)
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Paul Sleezer (B.S. '58)
Zachary K. Sweeney
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Sanford T. (Ph.D. '63) and Margaret Young

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Kimberly Estep (M.S. ’85, Ph.D. ’88)
Kenneth (Ph.D. ’60) and Susan Fahrenholtz (M.S. ’60)
Richard Fantazier (Ph.D. ’67)
David Haines Freeman (B.S. ’52)
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David J. Hart
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Siew Ho (B.A. ’80, B.S. ’80)
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Joan E. (B.A. ’64) and Alexander L. Johnson (Ph.D. ’64)
Anna Karrash (B.S. ’56)
Mark S. Kende
Matthew Kinzler (B.A. ’10, M.S. ’12)
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Bruce Szabo (M.S. ’89)
Anna Verderame (B.A. ’06)
Philip Gilbert Webb (Ph.D. ’70)
Paul Wermer (B.S. ’76)
Stephen Wrobleski (M.S. ’93, Ph.D. ’97)

CONTRIBUTIONS IN MEMORY OF...

Jack A. Kampmeier
Constance D. Harsh
Anne Kampmeier
Thomas Martini (Postdoc ’70)

Frank P. Buff
Alan M. Edelson `59 (B.S. ’59)

Annette D. Lee
Steven J. Lee (Ph.D. ’73)

MATCHING/CORPORATE GIFTS...

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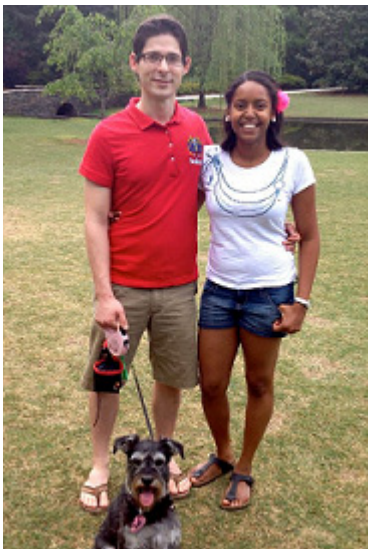
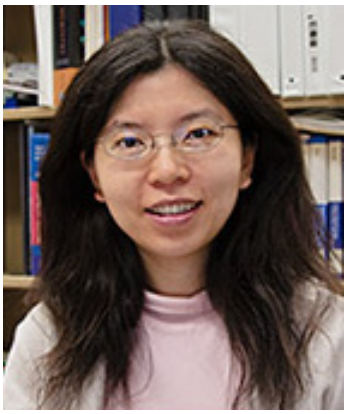
Alumni News

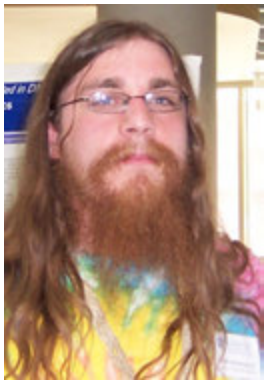


MATT MCLAUGHLIN (PH.D. '12, Holland group) and his wife, **KRYSTLE MCLAUGHLIN (PH.D. '12, BIOPHYSICS)** are enjoying their postdoctoral studies in the chemistry department at University of North Carolina at Chapel Hill (UNC-CH). Matt works in the Gagne group, focusing on developing new synthetic methods for complex bond constructions using transition metal catalysis, and won a National Research Council fellowship to fund his research. Krystle works in the Redinbo group on structural and biochemical characterization of proteins involved in the spread of antibiotic resistance. She is also a part of the SPIRE postdoctoral program at UNC-CH, having won a 3-year fellowship to support her research. As part of this program she will also be teaching at UNC-Pembroke in 2013.

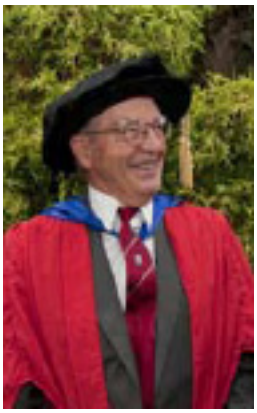
XIN WEN (M.S. '02, PH.D. '05), is being granted tenure and promoted to Associate Professor at California State university, Los Angeles (Department of Chemistry and Biochemistry) this fall. The research interests of Prof. Wen's group are at the chemistry-biology interface. They aim to understand the relationships between protein structure, dynamics, and function upon the ligand binding by biological, chemical, biophysical, and structural methods. Xin is especially grateful to Professor Kara Bren for all her guidance and support through the years.



RANDY MEHLENBACHER (B.S. '10) is currently a second year graduate student at the University of Wisconsin-Madison studying physical chemistry in the MARTIN ZANNI (B.A. '94, B.S. '94) group. He works on studying ultrafast energy transport processes in materials systems of interest for photovoltaic applications. He has already been on one paper (PNAS 2011;108:20902-20907. Adding a dimension to the infrared spectra of interfaces using heterodyne detected 2D sum-frequency generation (HD 2D SFG) spectroscopy Wei Xiong, Jennifer E. Laaser, Randy D. Mehlenbacher, and Martin T. Zanni, doi: 10.1073/pnas.1115055108). Randy received both the NSF (National Science Foundation) Graduate Research Fellowship and the NDSEG (National Defense Science and Engineering Graduate Fellowship) in the 2010-2011 competitions. He was forced to choose one and selected to be an NDSEG fellow.



GORDON A. NICHOLLS (POSTDOC '52) of Auckland, New Zealand has published his "Record of G.A. Nicholls Works," a copy of which may be checked out from the Carlsen Library here on the University of Rochester River Campus. His story spans thirty years, with twenty-six authors in three different countries, entailing an estimated 100 man-years of work (taking into account assistants, technicians and others).



SARAH (SALLY) SHEARD (B.A. '76) received a Ph.D. in Enterprise Systems (a field that concerns itself with how enterprises operate as a system, with [somewhat] predictable laws underneath the causes and effects) from Stevens Institute of Technology this past May, 36 years after beginning her first doctoral program at Cal Tech (she left with a Master of Science degree). In between she married, raised two children, moved to the Washington, DC area and held jobs as a high school teacher, satellite engineer, two jobs as a systems engineering consultant, and then formed her own company. She is currently a systems engineering consultant in the field of quantifying the impact of complexity on system development programs. An INCOSE (Interna-

tional Council on Systems Engineering) Fellow since 2006 and the 2002 INCOSE Founder's Award recipient, Ms Sheard has published over 30 INCOSE papers, led the Communications committee and the Measurement technical committee, and currently leads the Complex Systems working group. Sally still rides her bike and folkdances.

CLIFF KUBIAK (Ph.D. '80), received the ACS Inorganic Chemistry Award of 2012. This award aims to recognize and encourage fundamental research in the field of inorganic chemistry. In addition, recipients of this award must have accomplished outstanding research in the preparation, properties, reactions or structures of inorganic substances. The Kubiak research group at UCSD has three areas of focus: (1)"Ultrafast" electron transfer dynamic in organic mixed valence complexes, (2) molecular electronics and nanoscience, and (3) catalysis of atom transfer chemistry, especially the chemical and electrochemical conversion of carbon dioxide. Cliff was honored at the ACS Awards Ceremony in March in conjunction with the 243rd ACS National Meeting in San Diego, CA.

Clifford P. Kubiak (center) is presented his award by sponsor representative Josephine Nakhla (right) and ACS President Bassam Z. Shakhashiri (left).

MARK ROCHKIND (B.S. '62) returned to Rochester this year to commemorate his having graduated summa cum laude with a BS Chemistry fifty years ago. Mark went on to earn a Ph.D. at Berkeley, and returned to the University of Rochester to join the Department of Chemistry as an Assistant Professor in August 1965. A year later he joined the Chemical Physics Research Division of Bell Telephone Laboratories. During his career of 32 years, he spent 22 years at Bell Laboratories and AT&T and 9 years at Philips Electronics where he was President, Philips Laboratories (Briarcliff Manor, NY) and Executive Vice President of the Philips Lighting Group (Eindhoven, Netherlands). Mark now resides in New Jersey with his wife, Patricia.

CHIEN-HONG CHENG (Ph.D. '79) received the "Ho Chin Tui" Outstanding Honorary Award, created by the Hou Chin-Tui Foundation to reward high-achieving individuals in the field of fundamental science (including both physics and mathematics, and biology), material science, metallurgy, environmental conservation, and green building. Professor Chien-Hong Cheng, Department of Chemistry, National Tsing Hua University, is also the Vice President for Academic Affairs. Chien joined the Department of Chemistry in 1979 upon his return to Taiwan from Rochester. His work is divided between the areas of metal-organic chemistry—in which Prof. Cheng investigates and designs novel organic reactions catalyzed by metal complexes—and the design and fabrication of electroluminescent organic materials, with the ultimate goal of application to industry. Prof. Cheng's career has been highlighted by exceptional research results. In his research on reactions catalyzed by metal complexes, one of his selected papers explained the exchange reaction of aryl groups in palladium metal complexes with the aryl group in phosphorus ligands. This major discovery in metal-catalyzed reactions can be used to explain the creation of palladium by products at the end of catalyzed reactions. and was deemed significant enough to receive special publication in the American Journal *Chemtracts*.

SEBASTIEN FUCHS (POSTDOC '06) and wife, Stephanie - with now five-year-old Lois, decided to move closer to family in France and started a new job as GMP (Good Manufacturing Process) responsible in the company Tereos Syral, in Marckolsheim (centre of Alsace). Tereos Syral, a fast-growing company, is a leading producer of starch, starch sweeteners, alcohol and proteins in Europe. Tereos Syral processes natural raw materials (corn, wheat, potato and cassava) to manufacture a wide range of value added products in compliance with the current and future requirements of the food, pharmaceutical, green chemistry, animal nutrition, paper and corrugated board industries. Sebastien and family hope to visit Andrew Kende, C. F. Houghton Professor Emeritus of Chemistry, sometime in the near future.

Did you know . . we are on *youtube*?

www.youtube.com/user/UniversityRochester

The University of Rochester now posts the latest and greatest videos featuring students, faculty, and alumni, including our own **WALTER MOSS (Ph.D. '11)** with Professor Turner. Topic of discussion: "Is there an "off" switch for the flu?" Walter and his wife, Indee, have moved to Connecticut to start his postdoc at Yale. They are taking only their car and anything that fits in it to their 700 sq ft apartment!

Thanks to the volunteers, sponsors, and friends at the University of Rochester, the Kearns Center Upward Bound pre-college division was able to provide a successful summer program to their student population which largely consists of students from underrepresented minority groups in underperforming RCSD high schools. The students apply to Upward Bound for the academic support the staff offers during the academic year in their high schools. Over the summer, the Upward Bound students are bused to the River Campus, to give them a first-hand look at a college experience through coursework, college trips, and information sessions. This summer program's theme was oUR world - focused on bridging gaps between our local community and the global community. In the Chem E component of the introduction to engineering class, **ERIC NIELSEN (B.A. '11)**, co-taught with Kearns Center staff member Danielle Daniels, seeking to expose the students to something more hands on than just the periodic table of elements. Graciously, the Chemistry Department aided the students with space and supplies to set up a cosmetic chemistry laboratory, where the students were allowed to melt and mix their own lip balm. The lip balm lab was a success, and it was one of many projects and science labs that inspired more than a few young Upward Bound-ers to look at their studies in a different light. Eric began his medical school studies at the University of Rochester this fall.

IN MEMORIAM

The Department of Chemistry mourns the passing of:

- Carl W. Clarke (B.S. '62)
- Arthur H. Herz (B.S. '50, Ph.D. '54)
- Clare W. Johnson (B.S. '43, M.D. '46)
- Clifford E. Larrabee (Ph.D. '49)
- Bruce B. Love (B.S. '54, Ph.D. '61)
- Ruth Parker Oakley (B.A. '37, M.D. '41)
- Richard J. Rotondo (B.A. '49)

Interfaith Chapel

James M. Farrar Elected AAAS Fellow

James M. Farrar, professor of chemistry, has been elected a Fellow of the American Association for the Advancement of Science (AAAS) in recognition of his meritorious efforts in the advancement of science and its applications. The AAAS, an international nonprofit organization, is the world's largest general scientific society dedicated to advancing science around the world by serving as an educator, leader, spokesperson and professional association. In addition to organizing membership activities, the AAAS publishes the journal Science, as well as many scientific newsletters, books and reports, and spearheads programs that raise the bar of understanding for science worldwide. In the Chemistry Department here at the University of Rochester, Jim joins his colleagues, Robert K. Boeckman, Jr., William Jones, Thomas Krugh, Douglas Turner, and Richard Eisenberg as Fellows of the AAAS.

New fellows of the AAAS were presented with an official certificate and a gold and blue (representing science and engineering, respectively) rosette pin on Saturday, February 18th at the Fellows Forum, during the 2012 AAAS Annual Meeting in Vancouver, B.C. Jim was among 539 new members being honored for their scientifically or socially distinguished efforts to advance science or its applications.

Prof. Farrar was selected for his "distinguished contributions to gas phase ion chemistry, especially the dynamics of ion-molecule collisions and spectroscopy of mass-selected cluster ions." He received his Ph.D. from the University of Chicago in 1974 and joined the Rochester faculty two years later. Jim has taught many courses throughout his career, including physical chemistry and the large general chemistry courses, for which he received the Edward Peck Curtis Award for Excellence in Undergraduate Teaching (1985), the Goergen Award for Distinguished Achievement and Artistry in Undergraduate Teaching (2005), and election as the 2005-2006 Professor of the Year in Natural Sciences by the Students Association.

Farrar and his research group focus on reaction dynamics of ionic species. The objective of this research is to elucidate the reactivity of gas phase species important in electrical discharges, reactive ion etching, atmospheric and interstellar chemistry, and planetary atmospheres. The research also focuses on understanding processes involved in the transition from the gas phase to the condensed phases, as probed by spectroscopy through size-dependent properties of mass-selected cluster ions. The research employs the techniques of mass spectrometry, laser spectroscopy, molecular beams, and computation.

The present focus of the group is the application of the crossed beam method to studies of low energy ion-molecule reactions. The group has begun to apply state of the art imaging techniques for reconstructing product velocity space distributions by taking a snapshot of the spatial distribution of reaction products in a narrow time window. Reactions of current interest to the group include processes important in interstellar clouds and planetary atmospheres. The group's most recent publications have reported studies of the reactions of $C^+ + NH_3$, and N_2^+ and N^+ with CH_4. The latter reactions initiate ion processing in the atmosphere of Saturn's largest moon, Titan.

Jim and Toby

Fulbright Scholar Patrick Holland

Last year, Professor Patrick Holland was chosen as a 2011-2012 Fulbright Scholar. As a result, the Fulbright Foundation (a subsidiary of the U.S. State Department) gave him the financial and logistical support to support a four-month sabbatical in Mülheim an der Ruhr, a city in the northwest part of Germany. Here, he recounts his experiences:

The reason for choosing this location was the Max Planck Institute (MPI) for Bioinorganic Chemistry. One of the directors of this MPI is Prof. Frank Neese, a world leader in the application of computational methods to bioinorganic and organometallic chemistry. These techniques have revolutionized the understanding of molecular electronic structure, spectroscopy, and reactivity, and I would like to use these tools for my research on catalytically important coordination compounds. During this scientific "field trip," I gained a working knowledge of their techniques, submitted a couple of papers with them, and established the personal relationships that will support our continuing use of computational techniques. I also interacted extensively with Dr. Eckhard Bill, our longtime collaborator at the MPI.

In addition to doing research at the MPI, I traveled extensively, including Berlin, Zürich, Basel, Erlangen, Kiel, Regensburg, Bonn, Amsterdam, Leipzig, Cologne, Prague, Münster, Göttingen and London. Many of these jaunts were associated with a scientific conference or a visit to a university. I presented my group's research, gave tutorial lectures on nitrogenase and on crystallography, and even gave an invited lecture to the undergraduate students in the German Fulbright program. My travel allowed me to meet other scientists and also experience the interesting variety of culture, history, landscape, and food across Europe.

Pat and Maggie near Lake Lucerne in Switzerland

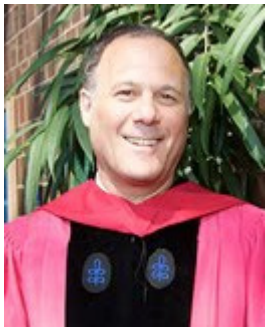
Pat Holland next to a monument to Heinrich Klaproth, the German chemist who discovered titanium, zirconium, and uranium

Of course, the motivations for spending time in Germany were not all scientific! The different language, culture, and customs were an enticing challenge for me and for my wife Maggie. Maggie is a faculty member in the School of Nursing at UR and was able to continue her research from Germany using the Internet for communication with coworkers and collaborators. During our time there, we made many new friends through the MPI, through our interests in music, and through "language partners" (Germans who seek out tandem language lessons with an English speaker). We each knew some German before our trip, and got plenty of chances to practice the language. Luckily for me, all of the science conversations were in English!

There were many aspects of living in Germany that were memorable. One example is the public transportation; it was easy to live without a car for four months. The food in Germany was amazing, and we will especially miss the fresh bread and white asparagus. The people in Germany were extremely gracious and welcoming, and we made friendships and memories that will last a lifetime.

Nature Chemistry | The Sceptical Chymist Reactions: Lewis Rothberg

This past June, Anne Pichon, Nature Publishing Group, contacted Lewis Rothberg, Professor of Chemistry, here at the University of Rochester, and subsequently published the following interview on The Sceptical Chymist blog. Lewis, also Professor of Physics and Chemical Engineering, works on the materials science underpinning organic electronics.



1. What made you want to be a chemist?

Since I learned about chemistry, I have always been excited by the idea of being able to explain macroscopic phenomena … things we see every day … with an abstract microscopic picture. In the interest of full disclosure, however, I am a physicist by training and passion even though my research is very chemical in nature.

2. If you weren't a chemist and could do any other job, what would it be – and why?

That's a hard one. I really love science and never looked back. Still, part of me wishes I could play professional basketball because I love the game and it looks like so much fun to be able to perform at that level. Another fantasy is facilitating innovation that would help Third World and impoverished populations by being a (philanthropically minded) venture capitalist. I'd also love to be a philosopher.

3. What are you working on now, and where do you hope it will lead?

My research group works on some of the barriers to wider application of organic electronics, materials stability, light extraction from LEDs, charge separation in photovoltaics, understanding the origin of apparent limitations such as spin statistics in OLEDs and aggregation quenching of luminescence.

4. Which historical figure would you most like to have dinner with – and why?

I'd like to meet St. Augustine – he seems to have grappled with many of the theological and moral problems at the core of the meaning of life with real grace and insight.

5. When was the last time you did an experiment in the lab – and what was it?

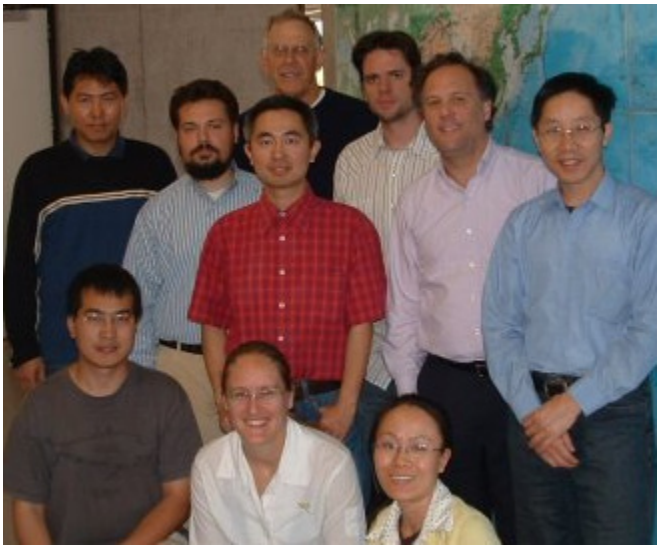
I do small experiments all the time and work in the lab with undergraduates a lot but in 2001 I worked on developing a new sensing approach to detect unlabeled analytes that is based on reflective interferometry. I was proud that this technology was patented and licensed by a small company interested in point of care medical diagnostics.

6. If exiled on a desert island, what one book and one music album would you take with you?

Vivaldi's Four Seasons always makes me feel joyous and hopeful. It may be hyperbole to say that nothing new has been said since Plato, but there seems to me enough truth in it that I would like to take a book of Plato's complete works.

7. Which chemist would you like to see interviewed on Reactions – and why?

I admire the chemists that have gone beyond taking on the big scientific issues and speak articulately on the importance of what we do to the public. … perhaps the most pressing technological issue we face is environmentally responsible and sustainable energy which looks like it has to come from sunlight and water in the very long run if we are to survive. I couldn't single out any particular chemist but Dan Nocera, Nate Lewis, Tom Mallouk …. The importance of this should inspire young people to go into science and development and understanding of improved and inexpensive catalysts (chemistry!) looks to me to be the most critical component of what needs to happen.



The Rothberg Group

Nanomaterials Symposium 2012

On Monday, May 21, 2012, the Rochester Advanced Material Program (RAMP) hosted the Nanomaterials Symposium on Frontiers in Materials Science for the 21st Century: Materials and Processes for Renewable Energy. This event was co-sponsored by the Hajim School of Engineering & Applied Sciences, and the School of Arts & Sciences. It is affiliated with the UR Integrated Nanosystems Center.

A signature challenge is the design of materials able to solve one of the great concerns of the 21st century: the harvesting, production, and use of energy in a sustainable manner. Six keynote speakers addressed the problem from several perspectives including discussions of photoactive materials, quantum-coherence in light harvesting, novel fuel cell materials, and nanometer scale materials. Contributed papers discussed energy and nanotechnological materials science research at the University of Rochester, as well as in the greater New York area. This all day, "Gordon Conference" style format allowed for much discussion and exchange of ideas.

The day began early with opening comments by Symposium Chair and Materials Science Program Director Todd Krauss. The first talk of the morning, "Plexcore® OC: Aqueous and Non-Aqueous Solution Processed HILs for Organic Electronics Applications," was given by Christopher Brown, Ph.D., Director of Technology, Materials at Plextronics, Inc. Chris Brown received his bachelor's degree in Biochemistry at the State University of New York at Stony Brook in 1990 and his Ph.D. in Chemistry from The University of Texas at Austin in 1997. After working as a research scientist and commercialization program manager at Eastman Kodak Company in the areas of photographic and OLED materials, he joined Plextronics Inc. in Pittsburgh, Pennsylvania in 2006 as a senior scientist in support of the OLED and OPV teams, and became Director of Technology for Materials.

From left: Lewis Rothberg, Christopher Brown, Michael Hickner, Todd Krauss, Richard Hennig, Kara Bren, Mitch Anthamatten, and Greg Scholes

Duncan Moore, Ph.D., Rudolf and Hilda Kingslake Professor in Optical Engineering with the Institute of Optics and Professor of Optics, Biomedical Engineering, and Business Administration in the Simon Graduate School of Business Administration, University of Rochester, spoke next on "Gradient-Index Optics and Concentrating Photovoltaics." Dr. Moore holds masters and Ph.D. degrees in optics from the University of Rochester, and a bachelor's degree in physics from the University of Maine. He serves on the Board of Trustees at the Rochester Museum and Science Center.

The morning talks ended with Richard G. Hennig, Ph.D., Assistant Professor of Materials Science and Engineering at Cornell University who discussed "Prediction and Design of Materials from Crystal Structures to Nanocrystal Morphology and Assembly." Professor Hennig received his Diploma in Physics at the University of Göttingen in 1997 and his Ph.D. in Physics from Washington University in St. Louis in 2000. After working as a postdoctoral researcher and research scientist at Ohio State University, he joined the faculty of the Department of Materials Science and Engineering at Cornell in 2006.

Lunch was followed by a poster session sponsored by the UR Chapter of the Materials Research Society (MRS). There were a total of eighteen posters representing many of the departments whose faculty are members of RAMP. Three of the poster session participants were selected by a committee of faculty and students to give a fifteen minute presentation about their research during the symposium. The poster presenters who were chosen to speak were Dr. Alexander Shveyd, a joint postdoctoral fellow with Prof. Lewis Rothberg, Prof. Ching Tang, and Prof. Shaw Chen; Heather Jaeger, a Ph.D. student in Prof. Oleg Prezhdo's group; and Supacharee Roddecha, a Ph.D. student in Prof. Mitch Anthamatten's group.

Afternoon talks began with Kara Bren, Ph.D., Professor of Chemistry, University of Rochester who spoke on "Bio-Nano

Constructs for Solar Fuels." Kara Bren received her BA in Chemistry in 1991 and her Ph.D. in Chemistry from Caltech in 1995. In 1997, she joined the faculty at the University of Rochester where she has been an Alfred P. Sloan Fellow, a Paul Saltman Memorial Lecturer, and an ACS/Dreyfus Lecturer.

Gregory Scholes, Ph.D., D.J. Leroy Distinguished Professor of Chemistry at the Institute for Optical Science and Centre for Quantum Information and Quantum Control, University of Toronto presented "Lessons from Nature about Solar Light Harvesting." Greg undertook his Ph.D. studies at the University of Melbourne, then spent time at Imperial College London as a Ramsay Memorial research fellow and pursued further postdoctoral work at the University of California, Berkeley. Dr. Scholes serves as an Editorial Advisor for New Journal of Physics and is a Senior Editor for the Journal of Physical Chemistry Letters.

The day was complete with Michael Hickner, Ph.D., Assistant Professor and Virginia S. and Philip L. Walker, Jr. Faculty Fellow in the Department of Materials Science and Engineering at the Pennsylvania State University speaking on "New Polymer Membranes for Redox Flow Batteries and Fuel Cells." Mike's research group has ongoing projects in new polymer synthesis, fuel cells, batteries, water treatment membranes, and organic photovoltaic materials.

We look forward to next year's spring conference!

Nuclear Power Plant Reflection

This past spring, Dr. Schröder arranged for students from the ANSEL (Advanced Nuclear Science Education Laboratory) class to visit the nearby Robert Emmett Ginna Nuclear Power Plant. This was an excellent opportunity to marvel at the infrastructure and technology involved with generating electric power that has become part our daily lives.

Our tour began with a visit to the on-site control room simulator, where an exact replica of the plant control room is used to train operators for handling any potential scenario that could occur during operation. It was amazing to learn that there are only four or five people in the room at a time, each of which are responsible for an extensive list of specific tasks. The amount of analog equipment still in the room was amazing, as the plant has been operational since 1970. Our tour guide and fellow University of Rochester Alumni, **Greg Jones,** informed us that changes to the control room are made only when necessary since they can only be made during a short refueling period that occurs every 18 months.

After the control room simulator, we went through a security checkpoint that was more thorough than any airport. This was understandable, given that the technology inside the facility must be well protected for the sake of national security and environmental monitoring. It was heartening to learn that average radiation dose on site is on par with natural background levels. In fact, we were told that the average worker receives a significantly smaller dose than a single CT scan. Much of the chemistry studied on site involves rigorous testing of the plant emissions to ensure that they pose no hazard to the environment or workers on site.

We were not given access to the part of the plant containing the nuclear reactor due to regulatory and safety concerns; however, we were given a detailed tour of the secondary facility containing the steam generator. This area was very hot, humid and loud, due to the massive machinery involved with pumping vast amounts of hot steam through the turbines. There was a vast network of pipes that wandered all across the facility, centralized around the gigantic steam turbine, whose vibrations were strong enough to unsettle my footsteps. It was fascinating to see all of the different types of people working in the plant: from welders, machinists and technicians to scientists, engineers, operators and administrators. It really does take a variety of skill sets to operate and maintain a power plant, even if it is one of the smallest reactors in the country.

Many thanks to our main contact and guide Greg Jones, as well as the others who assisted with the tour: Phil Gardner, Will Folgheraite, and Dave Barrett. This was an unforgettable opportunity to explore career opportunities involved with nuclear science. ~ Ben Hmiel

Carlson Library Expands Workshop Space

The Carlson (Science) Library has created two new spaces for small group learning. Over the last fifteen years Carlson Library has subscribed to online journals when they became available. Because of tight budgets, they have discontinued their print subscriptions (print JACS in 2010). Additionally they have bought digital copies of older journal issues. As a consequence, students, faculty and staff read the journal subscriptions from anywhere in the world using their computers.

Rather than continuing to store seldom used print journals, library staff consulted with faculty and students about how the space might be reconfigured. They chose to provide more individual and group study spaces in addition to those already available. Starting in 2010, specific journals were identified to be moved to the Annex offsite storage facility. Then Champion moving company was hired to transport the journals and help shift the remaining print journals into a tight configuration. Facilities staff took down the unneeded shelving and found new homes for it. With a designer from Sedgwick, new tables, chairs, and modular study rooms were selected with the workshop (Peer Led Team Learning) students in mind. During spring 2012, walls were painted and a new carpet was installed. This summer, the furniture arrived and was carefully laid out, including two modular study rooms, eight new computers, new tables, 52 new chairs (13% increase in overall seating for the library), 16 new carrels and reupholstered comfortable chairs. Students, staff and faculty have space to spread out their papers, plug their laptops in and focus. Rolling whiteboards are nearby for enhanced group communication. This comfortable space is quiet, free from distractions, yet convenient to classes and labs.

We invite you to come visit!

The 2012 Chemistry-Biology-Biophysics Cluster Retreat

The third annual Chemistry-Biology-Biophysics Interface Retreat was held on June 7-8, 2012. The Retreat started on the afternoon of June 7th with a talk by Prof. Ken Johnson (Roger Williams Centennial Professor of Biochemistry, Institute of Cellular and Molecular Biology, University of Texas at Austin) to an audience of about 75 people in the Class of '62 Auditorium in the Medical Center. The talk was titled: "Role of conformational dynamics in HIV reverse transcriptase nucleotide specificity and the evolution of drug resistance" and was partially funded as the second Vincent du Vigneaud Lecture. Dr. du Vigneaud was a UR graduate student who went on to win the 1955 Nobel Prize in Chemistry. The lecture was followed by a lunch in Evarts Lounge in Helen Wood Hall. The Retreat continued at 4:00 pm with a lecture by Dr. Muthiah Manoharan (Senior Vice President, Alnylam Pharmaceuticals) to an audience of about 60 in Hutchison Hall Room 473. The title was "Making Drugs out of siRNAs". These talks provided an appreciation of the interface between basic research and drug development.

The Retreat reconvened at the Staybridge Suites Hotel 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 informative "Career Panel Discussion," that included Ken Johnson, Ph.D., Muthiah Manoharan, Ph.D., Jeffrey Bemis, Ph.D. (Director of Clinical Studies, Litron Laboratories), Anne M. Schneiderman, Ph.D., J.D. (Patent Attorney, Harris Beach, PLLC), Mike Neidig, Ph.D. and Brendan Mort, Ph.D. (Director of Center for Research Computing, University of Rochester). Valuable advice was given on what employers look for when screening CVs and interviewing candidates. Comments were also made on the importance of finding a rewarding job and leading a balanced life.

The afternoon's scientific talks ranged from Mike Neidig's review of "Physical-Inorganic Chemistry of Iron in Biology and Catalysis" and of the novel instrumentation he has set up in the Chemistry Department to Arielle Butts' "Mechanistic Characterization of the Antifungal Activity of Toremifene in Cryptococcus Neoformans." Arielle is a Chemistry graduate student working with Prof. Damian Krysan in the Pediatrics Department, a collaboration possible at very few universities. The interface between basic science and drug development was represented further by Dave Condon from the Turner lab "Improving Computational Predictions of Locked Nucleic Acid (LNA) Molecular Dynamics: Benchmarking with Nuclear Magnetic Resonance Studies" and Dr. Enea Salsi from the Ermolenko lab describing single molecule studies of the "Structural Dynamics of Elongation Factor EF-G During Ribosome Translocation."

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 summer Research Experience for Undergraduates (REU) programs. The Retreat gave all participants a broad overview of research related to biology and an appreciation of interdisciplinary approaches.

Above: Michael Neidig, Jeffrey Bemis, Ken Johnson, Muthiah Manoharan, Brendan Mort, and Doug Turner. Included below: Anne Schneiderman.

Student Awards and Accolades

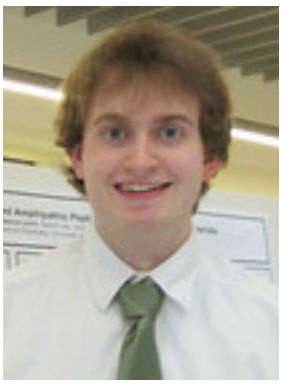
The Edward Peck Curtis Award for Excellence in Teaching by a Graduate Student is a University wide competition given to exceptional teaching assistants. **KYLE BIEGASEWICZ,** beginning his third year in Professor Boeckman's lab, was among the graduate students across the University who received the 2012 award. The nomination includes letters of support from the chair, faculty and students. Kyle is shown here at a department reception held in his honor.

Kyle Biegasiewicz receiving the Edward Peck Curtis Award for Excellence in Teaching by a Graduate Student

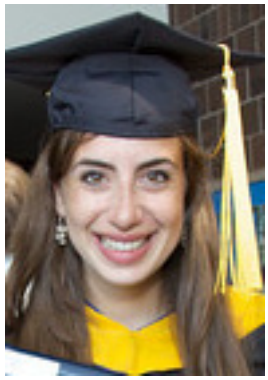
NSF Graduate Fellowships

Nine University of Rochester students and six alumni have been named recipients of the National Science Foundation Graduate Research Fellowships. Additionally, 18 current students and recent alumni also were given honorable mentions by the NSF. The fellowship, which is part of a federally sponsored program, provides up to three years of graduate study support for students pursing doctoral or research-based master's degrees. Since the program's inception in 1952, it has supported nearly 50,000 students conducting research in science, technology, engineering, mathematics, and selected social science disciplines. Of the more than 12,000 applicants, only 2,000 were awarded fellowships and 1,783 were given honorable mentions. The fellowship includes a three-year annual stipend of $30,000, a $10,500 educational allowance to the institution, and international research and professional development opportunities.

From the Department of Chemistry: **MARK LEVIN (B.S. '12**, Frontier Lab), **DAVID KAPHAN (B.S. '12**, Boeckman Lab), **KIMBERLY MANBECK** (1st-year grad student, Jones Lab), and **DAVID WEINBERG (B.S. '11**, Rothberg Lab). Honorable Mentions: **BENJAMIN SNYDER (B.S. '12,** Jones and Neidig labs), and **SAM ANDERSON (B.S. '11** Nilsson Lab, now at UNC Chapel Hill). Congratulations to all the awardees!



JONATHAN RAYBIN (B.S. '12), received the 2012 ACS Rochester Section Award and a Carl A. Whiteman, Jr. Teaching Award. Jonathan enjoyed his work with Professor Rothberg studying the photophysics of P3HT. He also worked as workshop leader for several chemistry and mathematic courses and as an editor for the Campus Times. He is continuing his education at the University of Chicago.



EMILY HART (B.S. '12), received the Presidential Award for Community Service, established by the Dean of Students in 1990 to recognize University students who are committed to community service. Given to a senior for outstanding participation and leadership in service to the community beyond the campus, this award recognizes a student who has worked selflessly and effectively in addressing social causes. Emily also won a Chemistry Department Award. This fall, Emily is teaching science in Brooklyn as a member of the 2012 Teach for America corp and is attending Fordham University to pursue a masters in secondary science education.

Chemistry major and Rochester Early Medical Scholar (REMS) **EMILY REDMAN (B.A. '12)**, received the Janet Howell Clark Prize. Established by the University, this award is given to the senior woman who has shown the greatest promise in creative work in one of the following fields - Physics, Chemistry, Biology, or Astronomy - and has shown outstanding versatility in the mastery of allied fields. Emily, who also received Department and Carl A. Whiteman, Jr. teaching awards, was

elected to both Phi Beta Kappa and Iota Sigma Pi Honor Societies as a junior. She is now the third woman Chemistry major in a row to win both the Catherine Block Memorial (junior year) and the Janet Howell Clark (senior) Prizes. She spent part of the summer in Europe before starting medical school here in Rochester this fall.

Each year the American Chemical Society (ACS) gives an Inorganic Chemistry Award to a student who is selected by the faculty on the basis of outstanding academic achievement in inorganic chemistry. **BENJAMIN SNYDER (B.S. '12),** this year's award winner, also received an honorable mention from the NSF Graduate Research Fellowship Program. After working with Professor Jones on a fellowship from the Center for Enabling New Technologies Through Catalysis and with Professor Michael Neidig as a visiting graduate student this past spring, Ben is pursuing a Ph.D. at Stanford University.

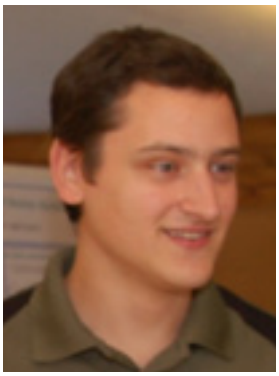
Ben Snyder, David Kaphan, and Mark Levin

Pictured with Ben is the John McCreary Memorial Prize winner, **DAVID KAPHAN (B.S. '12).** This prize was established in 1985 in tribute to the high academic and scientific standards, and the personal dedication of John James McCreary who received his B.S. degree in Chemistry in 1975. David has now started graduate studies with an NSF graduate research fellowship at the University of California, Berkeley. Joining him at Cal-Berkeley is **MARK LEVIN (B.S. '12),** winner of the Dr. E.W. and Maude V. Flagg Award. Mark has won numerous other awards while here at UR, including an honorable mention as a 2011 Barry M. Goldwater Scholar, being named an Amgen Scholar, which helped fund a summer research experience with the Toste Group at the University of California at Berkeley, a Merck Scholar Award, the ACS award for inorganic chemistry and election to Phi Beta Kappa, both as a junior. After spending several years in Professor Frontier's lab, he is pursuing a Ph.D. in organic chemistry funded by an NSF graduate research fellowship.

The Merck Index Award, given to a senior in recognition of outstanding intellectual accomplishment, including completion of a senior research project, went to **REBECCA LEVIN (B.S. '12),** who entered the Boston University Medical School this fall. Chemistry Department awards also went to **MATTHEW DEMARS, II (B.A. '12), KATHERINE KEIFER, (B.A. '12) AND PETER RICHTER (B.S. '12).** Peter was also the recipient of a Carl A. Whiteman, Jr. Teaching Award, as was **(FAYE GURA (B.A. '12).** Peter is attending MIT for research in physical chemistry.

Peter Richter

RYAN COWLEY (PH.D. '12), received a "Young Investigator Award" from the Inorganic Chemistry Division of the American Chemical Society (ACS). Ryan presented his Ph.D. research (with Pat Holland) at the 2012 Young Investigator Symposium given during the National ACS Meeting held this August in Philadelphia. This DIC symposium honors talented young inorganic chemists, and provides a high-profile forum for them to present their research results. Ryan is now pursuing postdoctoral studies with Edward I. Solomon (Stanford University) in physical bioinorganic chemistry, where he is investigating structure/function relationships in copper enzymes using spectroscopic and computational methods.



NAOMI LEE (graduate student in the Nilsson group and a member of the Armed Forces), received a travel award in 2012 to the American Indian Science and Engineering Society (AISES) national conference where she received an Honorable mention for graduate student oral presentations. Other travel awards went to **JOHN DIMAIO** (American Peptide Society, APS, summer conference), **RUJA SHRESTHA (PH.D. '12,** Graduate Research Symposium at UC Santa Barbara), and **WATHSALA LIYANAGE** (ACS Division of Organic Chemistry to the ACS national meeting in Philadelphia).

After having received an ACS travel award in 2011 and defending her thesis late in the year, **KAREN CHIANG (PH.D. '12),** joined her fiance, **ABDALLAH BITAR (M.D./PH.D. '09)** in San Diego, California. Abdallah is on the research track residency program at Scripps Green Hospital. Karen is pursuing internships and jobs related to science broadcasting.

This year the chemistry department only fielded one team, Hutch's Hitters, which was comprised of many returning members of last year's team as well as several prominent members of the now defunct Sheridan Shamrocks. The team was once again coached by **MICHAEL PRINSELL** and **MATT BETUSH** and made a fourth consecutive trip to the playoffs. Unfortunately, due to the timing of the Philadelphia American Chemical Society conference, we were only able to field exactly 10 members needed to not be shorthanded in our playoff game against the first place Rochester Rockets. Despite the valiant effort of players playing out of position, the team was not able to advance to the finals game and was eliminated in the first playoff game for the second year in a row. Hopefully next year we can not only return to the playoffs but return to the finals.

Hutch's Hitters

See also *Commencement* beginning on page 58

Laura Ackerman, Kyle Biegasiewicz, Lukiana Anka-Lufford, and Benjamin Hmiel at the 2012 Commencement Ceremony

Faculty News

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

rkb@rkbmac.chem.rochester.edu

During the 2011-2012 academic year, **ROBERT K. BOECKMAN, JR.** completed his ninth year as the chair of the chemistry department. Professor Boeckman is continuing as chair for a final one year term in 2012-2013 prior to the Chairmanship being assumed by Todd Krauss. 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 hydroxymethylation of aldehydes. Studies in this area are continuing toward asymmetric α oxidation of aldehydes and other applications. New collaborative projects have been initiated with Professors David Goldfarb of the biology department and Damian Krysan of the Department of Pediatrics, 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)** have moved to the Buffalo New York area where John is employed by the law firm of Hodgson Russ LLP in Buffalo, NY

Hutchison Hall

as a scientific advisor, and Yan Miller has been teaching at the University of Buffalo, and Buffalo State. **NATHAN E. GENUNG (PH.D. '10)** completed a postdoctoral stay with Larry Overman at UC Irvine and joined Pfizer Inc. in Groton, CT as a research scientist. **XINYI SONG (PH.D. '07)** continues to be employed as a research chemist with J&W Pharmlab in Levittown, PA. Matt Betush will soon be completing his research in the group on various aspects of asymmetric catalysis and will seek a teaching position. George Arab will complete his doctoral work on FK-506 in early 2013 and move to a postdoctoral appointment at Berkeley with Dean Toste. Brian Ohman left the group during the 2011-2012 academic year to take a position as an analytical chemist in a biotech firm in North Carolina. Part-time scientist Dr. Dennis Savage, retired from Kodak, continues his work in the group on several projects with the Goldfarb (biology) and Krysan groups (pediatrics URMC). Douglas Tusch and Kyle Biegasiewicz, now in their 2nd year, have just completed their doctoral candidacy exams. Doug has taken over apoptolidin from Brian Ohman, and Kyle is working with George Arab on FK-506. **DAVID KAPHAN (B.S. '12)** completed his B.S. thesis in the group in Spring 2012 and began graduate studies in chemistry at UC Berkeley this Fall. Gil Ryenders (Lake Forest College) joined the group in December 2011 and is working with Hui Wang on Nakadomarin A. **CHRISTINA COLLISON (PH.D. '04)** continues as associate professor of chemistry at RIT and **JEREMY CODY (PH.D. '04),** now assistant professor of chemistry also at RIT, will be considered for tenure in the Fall. **JOSEPH PERO (PH.D. '05)** continues as a research scientist with Merck in West Point, PA. **XIAORONG LIU (PH.D. '04)** continues as a research scientist at Astra-Zeneca in Waltham, MA.

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 saw many changes over the past year. Two graduate students, **WESLEY ASHER (PH.D. '12)** and **MEHMET CAN (PH.D. '12)** successfully defended their theses and took the next steps forward in their careers. Wes characterized the folding dynamics of single cytochrome *c* molecules in his thesis research, jointly advised by Kara and by Todd Krauss. In July 2012, Wes started a postdoc with Prof. Jonathan Javitch at Columbia where he is performing single-molecule studies of membrane proteins. Mehmet defended his thesis on determinants of electronic structure of cytochrome *c* variants and is now making use of his expertise as a postdoc with Prof. Stephen Ragsdale at the University of Michigan where he is performing spectroscopic studies of carbon monoxide dehydrogenase / acetyl-CoA synthase. Undergraduate thesis student **BENJAMIN SNYDER (B.S. '12)** wrapped up his work in the Bren lab and decided to pursue his Ph.D. studies in physical inorganic chemistry at Stanford University. With his double major in math and chemistry and extensive experience in spectroscopy, we are confident that Ben will shine in his chosen field. The group also bid farewell to three postdocs in the past year. **MATTHEW LIPTAK'S (POSTDOC '12)** research in the Bren group centered on NMR and DFT studies of heme conformation and electronic structure. He has now joined the chemistry faculty at the University of Vermont where he is establishing a research group in the area of metal tetrapyrrole biosynthesis and degradation. **ANDREA LEE (POSTDOC '12),** a joint postdoc with the Krauss lab, developed studies of single protein molecules at Rochester and is continuing studies of single-molecule biology at the University of Vermont Department of Microbiology and Molecular Genetics. **ANNI SIITONEN (POSTDOC '12)**, a joint postdoc with the Krauss lab, worked on nanotube

synthesis and interactions with cytochromes, and has moved to Boston and employment in industry.

Graduate student Jesse Kleingardner is holding the important role of senior student in the lab while continuing his work on two projects. In one, he is investigating heme conformation and electronic structure, and in the other he is developing metalloporphyrins as catalysts in collaboration with the Eisenberg lab. Jesse is also busy mentoring the group's two new graduate students, Becky Smith and Banu Kandemir. Becky started research on heme peptide conformation and electronic structure in the summer of 2011 and is continuing this project now. Furthermore, Becky is investigating effects of heme spin density distribution on electron transfer activity of cytochromes. Banu is developing photoactive proteins for electron transfer to hydrogen-evolving catalysts in collaboration with the Eisenberg lab, and is also participating in a collaboration with the Kristoffer Andersson group on electronic structure of cytochromes. Third-year student Lenore Kubie (joint student with the Krauss lab) is continuing her studies of charge transfer between porphyrins and nanotubes. As an IGERT student, she had the wonderful experience of traveling to Ghana in July 2012 to attend the I-SEE 2012 conference, to visit the Kwame Nkrumah University of Science and Technology (KNUST), and to teach 4th – 6th grade students (see picture p. 36). In the summer of 2012, incoming first-year student Leah Frenette joined Lenore's efforts on engineering nano-bio hybrid structures consisting of cytochromes and nanotubes. Also joining the lab in the summer of 2012 is undergraduate Benjamin Dick, who is working along with Jesse on engineering porphyrin-peptide conjugates.

Some Bren group alumni had exciting news. Undergraduate thesis student **RORY WATERMAN (B.S. '99)** was promoted to Associate Professor and awarded tenure at the University of Vermont. Former graduate student **BRANDY RUSSELL (PH.D. '03)** was promoted to Associate Professor with tenure at Gustavus Adolphus College in St. Peter, MN. Also, **SARAH BOWMAN (PH.D. '10**) accepted a position as Assistant Professor of Chemistry at the University of Minnesota at Duluth. Apparently, Kara has been successful promoting her home state to her students!

Kara had an eventful past year as well. She accepted positions on the Editorial Advisory Boards of *Accounts of Chemical Research* and the *Journal of Inorganic Biochemistry*. She also traveled to give eleven invited lectures at universities and at conferences. A highlight was the International Conference on Porphyrins and Phthalocyanines in beautiful Jeju, Korea in July 2012.

Rush Rhees from the front of the Eastman Quadrangle

Esther M. Conwell

Research Professor

Ph.D. 1948, University of Chicago

RESEARCH INTERESTS

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

CONTACT

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For **ESTHER CONWELL,** and others familiar with DNA, the discovery that an excess electron or a hole could move freely on a DNA stack suggested that DNA might be used to make, on a much smaller scale, devices of the type made with silicon and other semiconductors. For such devices to be of practical interest, however, an excess electron or hole would have to move many orders-of-magnitude faster than present measurements indicate they do. It aroused considerable interest, therefore, when it was announced recently that the speed of a hole on a series of adenines was increased by a factor of 130 when the adenines were replaced by deazaadenines, in which one of the electronegative nitrogens, N3 or N7, was replaced by a carbon and a hydrogen.

In an effort to understand hole motion on a series of deazaadenines (paired with thymines as in the experiments), we carried out calculations of the wavefunction of a hole injected into such a series. The calculations were carried out using the code CP2K, which we had used recently to simulate hole wavefunctions on a series of adenines paired with thymines. We calculated also for adenines with both N3 and N7 replaced by C-H. The resulting hole wavefunctions were found to behave similarly to those on the adenine-thymine chains: immediately after injection the wavefunctions were delocalized over some or all of the modified adenines (those where there was a water molecule within ~ 1.8A of the modified adenine did not acquire any of the hole wavefunction, presumably because of the formation of a hydrogen bond with N3 or N7 that repelled the hole). Within 20 fs or less, the hole wavefunctions were localized on a single one of the modified adenines, just as had been the case for the unmodified adenines. From the typical fs times for formation and breakup of the hydrogen bonds we concluded that they did not have any effect on the speed of hole motion. We concluded that the increased speed of the holes in the modified adenines is largely due to the decrease in the hole binding energy that results from removing an electronegative nitrogen.

The Susan B. Anthony Institute, the Susan B. Anthony Center for Women's Leadership, and the Rochester Center for Community Leadership organized a leadership panel as part of their Luncheon Series, in which Esther participated as an invited panelist, along with Lisa Norwood, Assistant Dean in the Hajim School of Engineering and Applied Science and KaeLyn Rich, Director of the Genesee Valley Civil Liberties Union. Angela Clark-Taylor of the Susan B. Anthony Institute facilitated the panel who reflected on their journeys to success in academia and non-profit work as well as answered questions.

In December of 2011, Esther received a Certificate of Appreciation for her "valuable contribution and dedicated service in the peer review of manuscripts submitted to ACS journals".

This year, faculty, family, and members of the department helped her celebrate her 90th birthday!

Joseph P. Dinnocenzo

Professor of Chemistry

Ph.D. 1983, Cornell University

RESEARCH INTERESTS

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

CONTACT

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JOE DINNOCENZO and his group continue to pursue a variety of problems in electron transfer and related chemistry. As part of an ongoing collaboration with Samir Farid, we are continuing to examine the dynamics of ground and excited state electron transfer reactions. We recently discovered that many of these reactions have a rate constant/driving force dependence that surprisingly follows a simple Sandros Boltzmann dependence. Our results contrast with a large number of previous electron transfer reactions where a gradual fall off of the electron transfer rate constants with the free energy of the reaction has been reported. We discovered that the discrepancies can be traced to a number of previously unrecognized factors, including, for example, the use of inaccurate redox potentials used in prior work and, for excited state electron transfer reactions, to the misassignment of the reaction mechanism, where the reactions were found to proceed through exciplex intermediates rather than by simple electron transfer. This requires that the latter reactions proceed by sequential partial electron transfers. It seems likely based on our work thus far that a large body of previously published data will need to be reinterpreted and new theories to model partial electron transfer reactions will need to be developed.

Two graduate students in Joe's group earned their Ph.D. degrees in the past year: **MARY LENCZEWSKI (PH.D. '12)** and **PU LUO (PH.D. '12)**. Mary's thesis demonstrated how the endocyclic restriction test could be successfully applied to determine the stereochemistry of nucleophilic substitutions on benzyltrialkyl-silane and -germane cation radicals. Pu's thesis work involved several projects, including understanding the mechanism for the unusual fragmenation 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. Pu also developed nanosecond redox equilibrium methods for determining accurate oxidation potentials for a wide variety of organic compounds and used these potentials to test a new model we are developing for understanding what controls the dynamics of electron transfer reactions. Mary is currently teaching chemistry at Bucks County Community College in the Philadelphia area. Pu was hired as a research scientist by Dow Chemical in Spring House, PA.

Joe is continuing research with graduate student Terrell Samoriski on a pedagogical research project involving the design, implementation, and evaluation of the Peer Led Teaming Learning (aka Workshops) model for CHM 210 (Honors Organic Laboratory II). A new graduate student, Adam Feinberg, joined the group this year. Adam is working on understanding the general mechanism for fragmentation of aryltrialkyl Group 14 cation radicals. Adam is also completely rewriting our computer programs to control new excimer and dye lasers that are being installed on the group's nanosecond transient absorption apparatus this summer.

Wilson Commons

Richard Eisenberg

Professor of Chemistry / Research Professor — Ph.D. 1967, Columbia University

RESEARCH INTERESTS

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

CONTACT

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The 2011-'12 year began in the glow of last year's celebration of Rich Eisenberg's career and his retirement from teaching, but proved instead to be "refirement" with more activities and travel than in previous years. One activity required three trips to Israel to complete (June and December, 2011 for two weeks each, and July, 2012 for four days). The work in Israel involved a committee that Rich chaired for the government's Council of Higher Education to evaluate all of the higher degree granting programs in Chemistry and make recommendations for improvement. Rich was joined in this effort by Al Bard (Texas), Tobin Marks (Northwestern), Bill Jorgensen (Yale), Joan Valentine (UCLA) and David Milstein (Weizmann). Reports were written for all of the institutions visited, as well as a general report, and it was gratifying to learn recently that the committee's recommendations have been endorsed by CHE and that adoption of suggested changes will be undertaken. It was a stimulating committee activity (truly!) with good falafel on the side.

David Milstein, Bill Jorgensen, Rich Eisenberg, Joan Valentine, Tobin Marks, Al Bard

Other travel focused around meetings and lectures at different universities. In August, the 50th anniversary of Inorganic Chemistry was celebrated at the Denver ACS Meeting with a five session symposium and a special dinner for participants and guests. The journal continues to thrive with the latest ISI report showing IC to have the greatest number of citations and the highest impact factor in its category for the primary reporting of new science (as opposed to review journals). Another of Rich's activities for the anniversary was a series of interviews that he conducted with leaders in inorganic chemistry that are freely available on the web (http://pubs.acs.org/page/inocaj/multimedia/voices.html). The last of these turns the table with Rich being interviewed by IC Associate Editors Jim Mayer and Bill Tolman. Overall, the interviews have been well received, and Rich would enjoy any comments you may have about them. He is especially gratified by teachers who say they have used the interviews in their college and high school courses with positive results.

In September, Rich and Marcia traveled to Crete where Rich lectured at the BioSol (Bioinspired Materials for Solar Energy Utilization) Conference for sustainable energy. Rich and Marcia were able to enjoy the conference and the beautiful setting with fellow participant Harry Gray and his wife Shirley. From Crete, the Eisenbergs traveled to Berlin to lecture at Humboldt University and then continued to the University of Zurich to do likewise. A particular treat at the University of Zurich was to see the original complexes prepared by Alfred Werner and his students - and to see just how meticulous and correct they were in the formulation of these compounds.

Some of Alfred Werner's original cobalt complexes

In October, Rich was in Delhi, India where he was a plenary lecturer at the Asian Conference on Coordination Chemistry. At the meeting, Rich had the good fortune to see **CHIEN-HONG CHENG (Ph.D. '79,** chcheng@mx.nthu.edu.tw) who studied with Rich in the late 1970's and who is now Professor of Chemistry and Vice-President for Academic Affairs

at National Tsing-Hua University in Taiwan. Further travels included the ACS Editors Conference in early January in San Diego, the CCI Solar Retreat and Advisory Board Meeting in Huntington Beach later that month, and a return to San Diego in March for the ACS Meeting during which Rich helped **CLIFF KUBIAK (Ph.D. '80)** celebrate his receipt of the 2012 ACS Award in Inorganic Chemistry. Cliff is the first Rochester alum to receive this great honor.

However, prior to the ACS Meeting there was a special occasion in Pasadena as Rich, Marcia and friends prepared to celebrate the big 7-0 (actually Rich and Marcia are watching our friends take the plunge first including Bob and Helen Grubbs, Maurice and Mary Huges Brookhart, Bob and Wendy Bergman, and Chuck and Martha Casey). It was a great time with a little Blue Suede Shoes and Dancin' in the Streets!!

The Eisenberg group continues to make progress developing and analyzing new systems for the photogeneration of H_2 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 during the past year was

Staring at the big "7 – 0" (sound track available on request)
From left: Wendy Bergman, John Bercaw, Martha Casey, Chuck Casey, Bob Bergman, Bob Grubbs, Helen Grubbs, Maurice Brookhart (the really tall guy – NOT), Marcia, Cliff Kubiak, Mary Hughes Brookhart, Rich

spear-headed by postdoctoral researchers Bill McNamara and Will Eckenhoff 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 H_2 generation. On iridium catalysis of electrocyclization reactions in a joint project with Alison Frontier, articles were published on research by graduate student Tulaza Vaidya who completed her Ph.D. work in June.

There was another change for Rich and Marcia during the past year in that they were able to escape the Rochester winter for several months in Sarasota, FL when they were not traveling. The entire family joined them in Sarasota for Thanksgiving and an extended family vacation took place in Turks and Caicos in February for the fifth time. Both granddaughters, Michayla and Isabella, are becoming superb swimmers.

There were significant group comings and goings during the past year including (1) the departure of postdoc **BILL MCNAMARA (PH.D. '12)** who did great research for two years and is joining the faculty of William and Mary College in Williamsburg, VA; (2) the graduation of **TULAZA VAIDYA (PH.D. '12)** who is now beginning a postdoctoral position at Cornell; (3) the arrival of postdoc Will Eckenhoff from Duquesne who has received an NSF Postdoctoral Fellowship for work on new catalysts for light-driven hydrogen generation; (4) a sabbatical visit by Prof. Wenfu Fu from the Technical Institute of Physics and Chemistry (CAS) in Beijing, PRC; and (5) the commencement of work by new graduate student Ryan Cheng from Brandeis University who will work on electrophilic catalysis of organic reactions in the joint project with Alison Frontier. Rich is also delighted to have a number of undergraduates (Ali Hamlin, Luxi Chen, Madeline Yin, Hyun-Uk Kang, Troy Wang and Mike Olezeski) working in the lab; they keep a steady stream of questions and a great level of activity in the laboratory. As stated at the start, this sure sounds like "refirement".

Samir Farid

Research Professor

Ph.D. 1967, Göttingen University

RESEARCH INTERESTS

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

CONTACT

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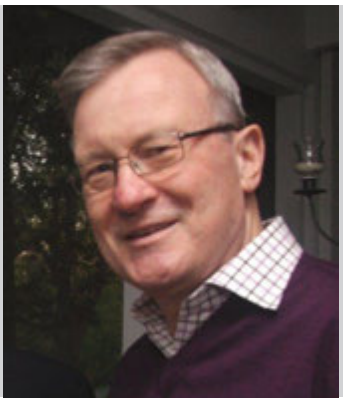
SAMIR FARID is currently working on two problems: photochemical chain amplified reactions and electron transfer kinetics. The work on chain amplification is carried out in collaboration with Deepak Shukla (Eastman Kodak). It explores reactions of alkoxy radicals with pyridine bases, which lead to quantum yields in the hundreds. Work on the steric effect on electron transfer kinetics has been concluded and appeared as a Featured Article in the *Journal of Organic Chemistry*. It showed that steric hindrance prevents the reactants from approaching an optimal configuration for electron transfer to occur, which weakens the electronic coupling and decreases the electron transfer rate constants by as much as an order of magnitude. The work on electron transfer kinetics is now focusing on the effect of increasing the reorganization energies. As usual the most enjoyable aspect continues to be the collaboration with Joe Dinnocenzo and Ralph Young.

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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This year has been a good one for **JIM FARRAR** and his research program. The group's first paper on ion imaging, published in the *Journal of Chemical Physics*, was selected by the editors as a Research Highlight, and was one of the top 20 papers downloaded in June 2012. Jim thinks three people downloaded the paper. Postdoc Linsen Pei continues his excellent work on the project, and our next challenge is to carry out studies of ion reactions with free radicals. Stay tuned.

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

Although Jim's research group has remained fixed in size, his family has grown recently, with the birth of granddaughter Josefina Emilia to his daughter-in-law and son in Jersey City. Jim and Kathy continue to make many trips to the New York City area to visit children and grandchildren.

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.

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It has been an exciting and eventful year for **RUDI FASAN** and his group. Significant steps forward have been made in our projects related to the development of P450-based methodologies for selective sp3 C—H functionalization. Assisted by UR undergraduate Brian Shafer and **MATTHEW DEMARS II (B.A.'12),** Kaidong Zhang (post-doc) established a general method for P450 reactivity prediction via P450 fingerprint multivariate analysis and provided a first demonstration of the potential of this approach by developing a set of highly regio- and stereoselective P450 catalysts for the hydroxylation of three isolated C—H sites in artemisinin. These P450 catalysts open the way to the late-stage functionalization of this complex natural product at positions previously inaccessible by conventional chemical methods. A full paper describing this work was just recently accepted for publication in the *Journal of the American Chemical Society*. **JOSHUA KOLEV (M.S.'12)**, who successfully passed his Ph.D. candidacy exam in July, is now exploring the scope of this methodology in the context of the anticancer sesquiterpene lactone parthenolide. Important progress has also been achieved in our MOrPH-related projects. John Frost (third-year graduate student), Francesca Vitali (post-doc), and UR undergraduate Nicholas Jacob ('13) recently completed an interesting set of studies to explore the mechanism and structure-reactivity relationships for the macrocyclization of organo-peptide hybrids via a dual, catalyst-free ligation approach. A first paper on the methodology appeared in *Chemical Communications* earlier this year, whereas a second manuscript focused on this later work is currently under review. The group has also been active in seeking intellectual property protection on inventions made in the laboratory. This year we filed two patent applications, one covering our methodologies for MOrPH synthesis (with Jessica Smith (fourth-year graduate student), John Frost, and Francesca Vitali (as co-inventors) and a second one focusing on our methods for P450 fingerprinting and fingerprint-based reactivity prediction (with Kaidong Zhang as co-inventor). Another very exciting event of this year was the funding of our first R01 grant by the National Institutes of Health. This $1.4M grant will support our P450-centered projects for the next five years. We are thankful to NIH as well as the

Fasan Group, Summer 2012

National Science Foundation and the University of Rochester Provost's Office (2011 Multidisciplinary Research Award) for their continuing support to our research efforts.

Several group members contributed to disseminate our research findings at various conferences across the country. Rudi presented recent accomplishments of the group at the XXI Enzyme Engineering Conference in Vail, CO, at the Gordon Research Conference of Biocatalysis, and at the Gordon Conference of Bioorganic Chemistry. Kaidong attended the latter as well, presenting a poster on the artemisinin project. Jessica Smith gave an oral presentation at the 243rd American Chemical Society National Meeting in San Diego, CA. John Frost and Josh Kolev spoke at the 2012 ACS Fall Meeting in Philadelphia, PA. John also visited Canisius College, from which he graduated in 2009, to give an invited seminar on his current research. Our younger, undergraduate students did an equally great job in representing the group at national and regional meetings. Kudos to Nicholas Jacob ('13) and **MATTHEW DEMARS II (B.A. '12)** who were selected to give a talk about their senior research projects at the 2012 Western New York ACS Section Meeting in Buffalo, NY, and at the 2012 National Conference of Undergraduate Research (NCUR) at Weber State University in Ogden, UT, respectively.

Other notable news concern the various awards bestowed to the group members in recognition of their research and/or scholarly accomplishments. Our congratulations go to Jessica Smith for receiving a Hooker fellowship and a Eli Lilly Travel Award to attend the ACS meeting, to John Frost and Josh Kolev for the award of a Sherman-Clarke Fellowship, to Louis Papa ('14) for receiving a Merck Index Award, and to Philip Cistrone ('13) for being selected as a recipient of a De Kiewiet Fellowship.

In terms of new additions, the lab has continued to attract a number of talented UR undergraduate students who have carried out independent research within a variety of synthetic and protein chemistry projects. These include Tatyana Dyndikova ('13), **MARYAM MOHAMMED (B.A. '12)**, Philip Sutera ('14), Louis Papa ('14), Philip Cistrone ('13), and Nicholas Hill ('15). We also enjoyed having McNair fellows Chandra Ade-Brown and Yick Chong Lam and REU fellows Peter Krasniak and Zachariah Hale, who conducted research over the summer. As new students come in, some current and former lab members have completed their undergraduate studies this year and get ready for their next step in their career. We wish best of luck to **MATTHEW DEMARS II (B.A. '12)**, who joined the Chemical Biology Ph.D. program at the University of Michigan in the Fall, **MARYAM MOHAMMED (B.A. '12)**, who joined the M.D. program at the Medical School of the University of Chicago, and **BRIAN SHAFER (B.S. '12)**, who was admitted to the Temple University School of Medicine.

In Spring, Rudi enjoyed teaching for the first time the course in Biological Chemistry (CHM 262/462), introducing peer-led workshops into the course. He was also engaged in a number of synergistic activities throughout the year, such as contributing an invited review to ACS Catalysis (which made the journal cover for the April issue), serving as grant review panelist for two programs of the National Science Foundation, and co-organizing a symposium on C—H activation for the 2013 ACS Spring Meeting in New Orleans.

On the personal side, a major, life-changing event in Francesca's and Rudi's lives was the birth of their first child, Penelope Iris Fasan, on February 16.

Flowers near Hutchison Hall

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. In our laboratory, the study of Nazarov cyclization began with evaluation of a new paradigm for designing precursors for Nazarov cyclization, which led to efficient catalytic Nazarov cyclization. Since those early studies, we have identified alternative starting points for the cyclization, and observed rearrangement chemistry that competes with the expected cyclization pathway. In the past year, our understanding of electrocyclic/ cationic/ cascade reaction sequences combined with some new discoveries has led to the study of other types of cyclization cascades. Joint studies with Rich Eisenberg have expanded from Ir(III) catalysis to gold catalysis, and our study of conjugate addition initiation of Nazarov cyclization has revealed unusual reaction pathways that will be the subject of future study. Work on asymmetric cyclizations and applications of Nazarov cyclization toward total synthesis of natural products continues.

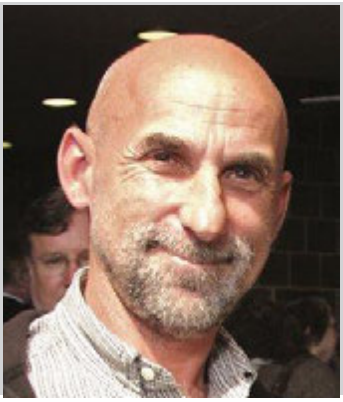
This year, we welcome Ryan Cheng, a graduate of Brandeis University, to the group. He is a joint student with Rich Eisenberg. We also congratulate **TULAZA VAIDYA (PH.D. '12)** and **JENNIFER CIESIELSKI (PH.D. '12)**, who both earned their Ph.D.s this summer. Tulaza will remain in the Western NY neighborhood, pursuing postdoctoral studies at Cornell University with Professor G. Coates, while Jen will relocate to the ETH in Zürich, Switzerland and work with Erick Carreira as an NSF postdoctoral fellow. **DR. DAVID LEBOEUF (POSTDOC '12)** finished his postdoctoral studies in the group in the spring, and will conduct additional postdoctoral studies under the tutelage of Professor Antonio Echavarren in Tarragona, Spain.

Over the past few years, Tulaza Vaidya (fifth-year student, working jointly with Rich Eisenberg) has developed remarkably active Ir(III) complexes as Nazarov cyclization catalysts. This year, she discovered a new gold catalyst that has remarkable reactivity for Nazarov cyclization and other cationic transformations. Ryan Cheng (first-year student) will continue her work. Our studies on different classes of cationic rearrangements (Nazarov cyclization/ [1,2] Wagner-Meerwein rearrangement sequence) continued this year (Eric Theiste, fifth-year student; and Dr. David LeBoeuf). In collaboration with Professor Vincent Gandon, of the Institut de Chimie Moléculaire et des Matériaux d'Orsay, in France, David demonstrated that DFT is an effective computational method for evaluating rearrangement pathways and predicting chemoselectivity in these reactions. We defined three factors that factor into rearrangement selectivity, and demonstrated our ability to predict (using DFT) and/or control (via substrate design and/or catalyst choice) these complex reaction sequences. A different type of multistep reaction sequence is under investigation by Josh Brooks (third-year student), who has expanded upon his studies of conjugate addition-initiated electrocyclization. This year, he discovered several remarkable cyclization cascades catalyzed by DABCO. In these sequences, it is possible to begin with a relatively simple, but also unusual dienyl diketone reagent, add a tertiary amine (DABCO was optimal), and execute highly efficient, diastereoselective reaction sequences. Josh has shown that these novel reactions create complex fused ring systems using a robust protocol that is scalable and air- and water-tolerant. Further studies in this area are underway.

In our natural product synthesis studies, Jen Ciesielski achieved a synthesis of the challenging tricyclic oxadecalin core of phomactin A, using a novel cyclization cascade strategy involving a β-iodoallenolate intermediate. Dr. David LeBoeuf completed a total synthesis of enokipodin B using our Nazarov cyclization/ rearrangement sequence. In an exciting continuing story, Peter Carlsen (third year student) continues to improve upon our cyclization strategy for the diastereoselective synthesis of tetrapetalone A. Finally, inspired by 1) the results of Dr. Craig Jordan and his group (URMC), who are finding that the natural product rocaglamide has unique properties as a agent for the destruction of leukemia stem cells, and 2) our interest in the Nazarov cyclization, Steve Jacob has embarked upon a second-generation strategy of this challenging target.

Joshua L. Goodman

Professor of Chemistry — Ph.D. 1984, Yale University



RESEARCH INTERESTS

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

CONTACT

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JOSH GOODMAN'S research interest is on the investigation of organic reaction mechanisms using a variety of time-resolved techniques such as pico- and nanosecond absorption spectroscopy and photoacoustic calorimetry. In particular, they have been examining processes in which electron transfer is coupled to bond breaking, and/or bond making. These bond-coupled electron transfer (BCET) reactions have the potential to drive chemical reactions using light. They have focused primarily on dissociative return electron transfer (DRET) reactions that involve cleavage of C-C, Si-Si and Ge-Ge bonds.

Entrance to Hoyt

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 group had an exceptionally good year in 2011-2012. One of the highlights was a publication in *Science* that described the first example of an iron complex that breaks the N-N bond of N_2. This was the work of **MEGHAN RODRIGUEZ (PH.D. '12)**, who also published a paper in *Angewandte Chemie* on the first iron-sulfide complexes with the iron in the unusually low iron(I) oxidation state. Meghan graduated with her Ph.D. in the summer of 2012, and plans a future in teaching.

She is one of five Ph.D. graduates from the Holland group within the 2011-2012 season! The others were all extremely successful as well. **MATT MCLAUGHLIN (PH.D. '12)** completed his thesis, which led to one paper this year in *Inorganic Chemistry* and two more publications are anticipated. Matt is now pursuing postdoctoral research with Mike Gagné at UNC Chapel Hill. **RYAN COWLEY (PH.D. '12)** finished his work on iron(III) imido complexes, which earned him a Young Investigator Award from the Division of Inorganic Chemistry of the ACS: this is very prestigious, as there are only eight awardees nationally every year. Ryan is now a postdoc with Ed Solomon at Stanford University, and recently was the chairman of the Gordon Research Seminar on Inorganic Chemistry. **KAREN CHIANG (PH.D. '12)** completed her research on highly reduced iron(I) hydride and aryloxide complexes, and the former has already appeared in *Angewandte Chemie*, where

The Holland Group

it was labeled a "Hot Paper." **THOMAS DUGAN** (PH.D. '12) also wrote an outstanding Ph.D. thesis, and one of the publications was a *J. Am. Chem. Soc.* communication on a very unusual cobalt(I) complex and its reactions. Tom is now a postdoc with Alan Goldman at Rutgers University. These students formed a tight-knit group that has been incredibly successful over the past few years, and it is both sad to see them go and inspiring to look forward to their great futures.

We also bid goodbye to **JONATHAN GOLDBERG (B.S. '12)**, who was an outstanding undergraduate researcher in the group for two years and a major contributor to a paper that recently appeared in a special issue of *Organometallics* on fluorine chemistry. Also, **P. M. GURUBASAVARAJ (POSTDOC '12)** returned to India, and graduate student **WENWEN YAO (M.S. '12)** graduated with her Masters degree and returned to China for a chemistry career. **WILLIAM MCNAMARA (POSTDOC '12),** who was joint with the Eisenberg group, has moved on to a faculty position at the College of William & Mary in Virginia. We wish all of them the best fortune in the future.

To balance these departures, we have new group members that will be providing the next wave of research in the group. New postdoctoral associates are Katarzyna Grubel, who comes from a Ph.D. at Utah State University, and Cory MacLeod, who comes from a Ph.D. at the University of British Columbia Okanagan. New graduate students are Malik Al-Afyouni, Megan Reesbeck, and Nicholas Arnet. Malik is further developing our cobalt compounds, and Nick, Megan, Kasia, and Cory will be pushing the envelope of our iron-sulfide and iron-N_2 chemistry.

Our joint project with the Eisenberg group has been extremely productive, with several papers describing novel homogeneous systems that use light to drive the production of H_2 from protons. Zhiji Han was awarded an Elon Hooker Fellowship in recognition of his outstanding research accomplishments in this area. We also have collaborations with the Krauss, Bren, Weix and Neidig groups within the department, and numerous outside collaborations as well. We have an exciting new collaboration with Chaim Sukenik at Bar-Ilan University in Israel, which will include student visits over the Atlantic in both directions.

Pat gave ten invited lectures in the U.S., two in Israel, and eight in Germany this past year. The ones in Germany were enabled by a Fulbright grant and a sabbatical leave from UR during the spring of 2012. This sabbatical travel also gave Pat the opportunity to learn more about computational chemistry, and to keep pace with Sarina Bellows, a fourth-year graduate student in the group who has become a computational chemistry aficionado.

In alumni news, **BRYAN STUBBERT (POSTDOC '07)** is now at Dow Central Research in Midland, MI, and **TRAVIS HEBDEN (B.S. '04, MASTERS '05)** moved to Intel in Portland, OR. **BEN GILSTON (B.S. '05)** has defended his Ph.D. thesis at Northwestern University. **EMILY BONES (B.S. '01)** is now an Assistant Editor at *Chemical & Engineering News*. **BEN DIBLE (POSTDOC '06-'09)** is the proud father of a new "coupling product" (this guy never stops thinking about catalysis!).

William D. Jones

Charles F. Houghton Professor of Chemistry Ph.D. 1979, California Institute of Technology

RESEARCH INTERESTS

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

CONTACT

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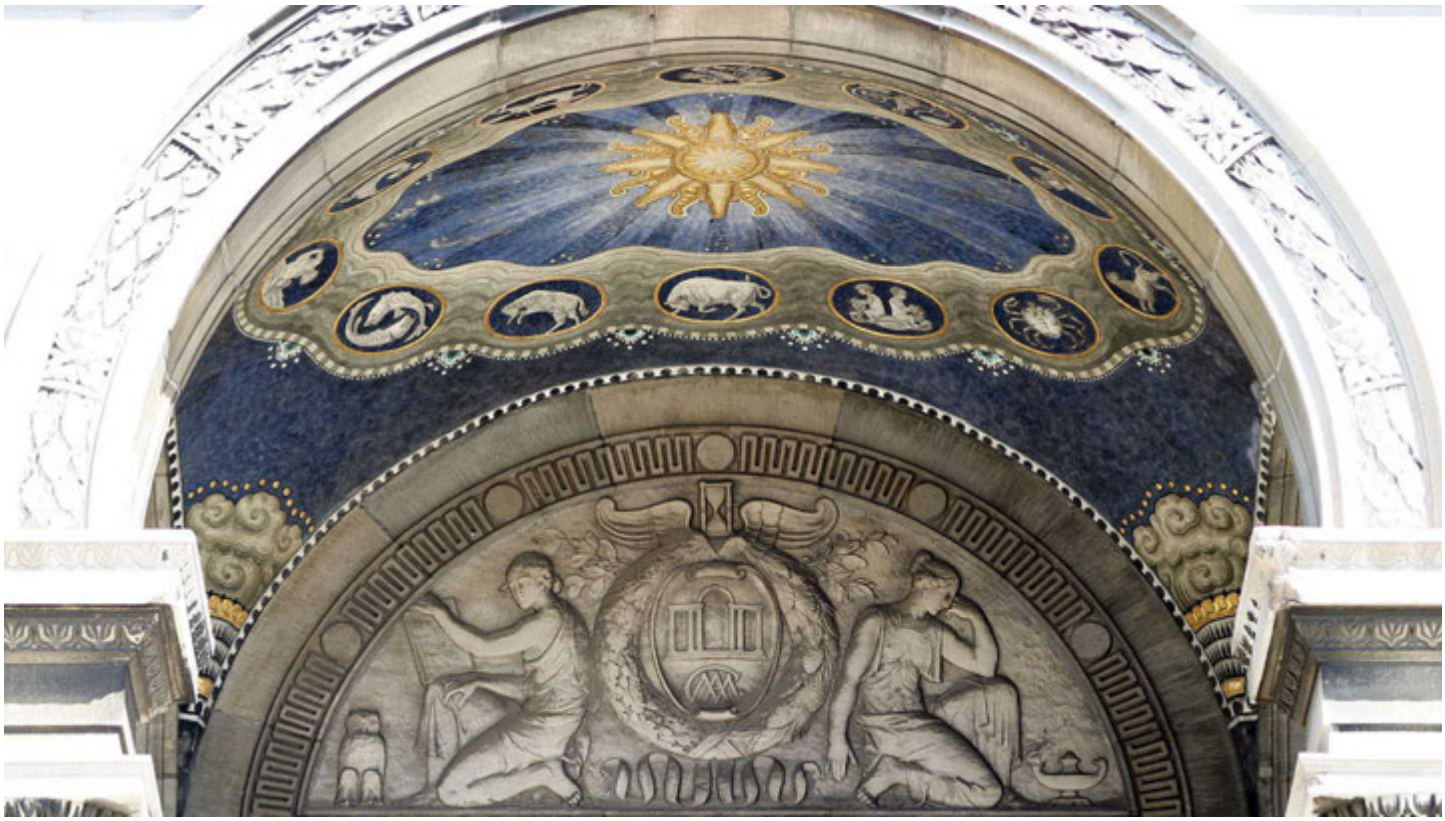
The **BILL JONES** group continues to actively pursue organometallic chemistry and catalysis. We had one new graduate student join the group this year, Lloyd Munjanja, and we have a visiting student from China, Juanjuan Li, for one year. Dr. Ruth Rodrigo joined the group in January 2012 following her Ph.D. work with Miguel Esteruelas in Zaragosa. Also, Gyeongshin Chen finished a four month visit with the group from Mashima's lab at Osaka University. The lab has nine people now, and renovations were undertaken in the spring that combined rooms B42 and B46. We now have four new 8-ft. hoods and a lot more instrument space! Our research is examining the activation of C-H bonds in substituted hydrocarbons, the cleavage of carbon-carbon bonds in alkynes and nitriles, and the C-S cleavage/hydrogenation of thiophenes. An important advance this year has been the elucidation of factors that control metal-carbon bond energies, such that we can now predict which products will be favored in a variety of reactions. These projects have involved a variety of fundamental studies of model reactions, as well as actual catalysis. The group continues its role in the Center for Enabling New Technologies through Catalysis (CENTC), in which the group has collaborative research projects that are exploring new electrophilic C-H activation catalysts and new direct routes to aromatic amines from benzene. Bill continues as Associate Editor for the *Journal of the American Chemical Society* for a ninth year, where he handled close to 500 manuscripts last year. He lectured in/at Toronto,

Archway - Eastman



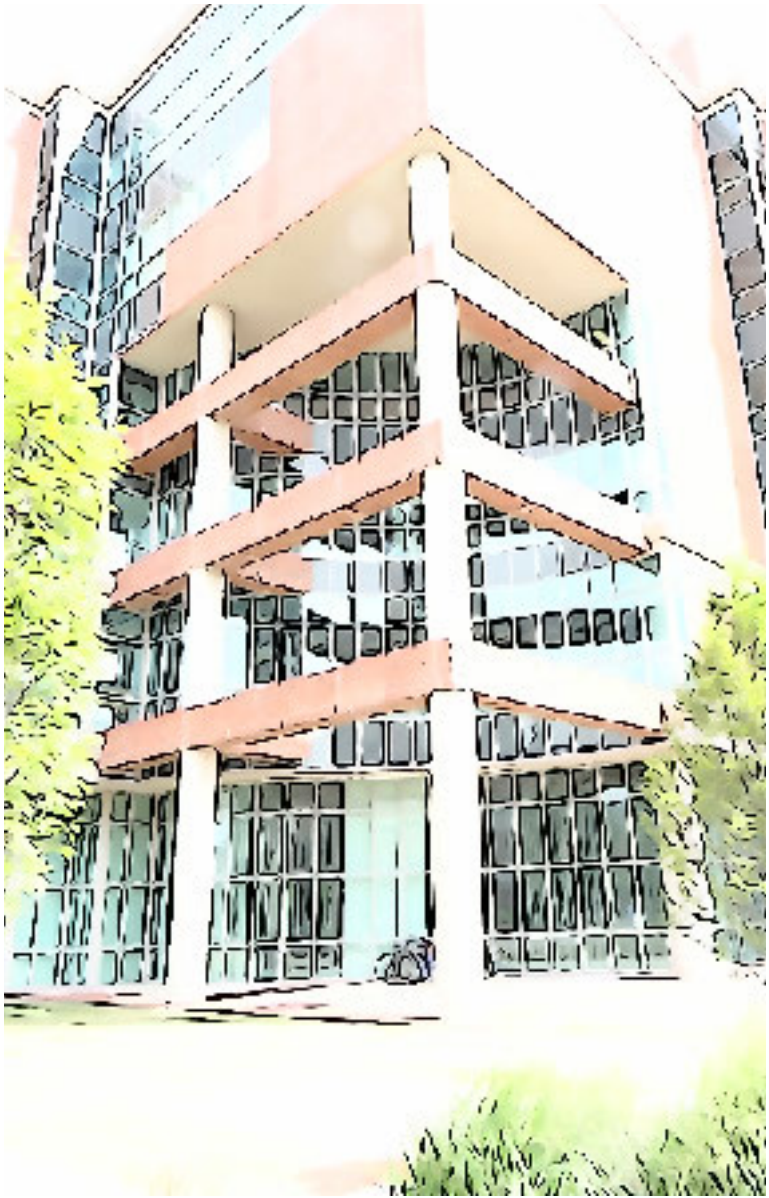
San Diego, Chinese Academy of Sciences, Shaanxi Normal University (Xian, China), Castellon (Spain), Toulouse (France), and Lisbon. Bill also gave two lectures in a special short course on fluorine chemistry at the Free University of Berlin and the Humboldt University. He also was the John Osborn Lecturer at the University of Strasbourg in April. Two graduate students completed their degrees, , **JENN RHINEHART (PH.D. '11)** and **MEAGAN EVANS (PH.D. '11)**. Jenn is now postdocing at the University of Tennessee with Prof. Brian Long. Meagan completed a postdoc with Rich Jordan at Chicago, and recently started a new position at Exxon-Mobil in Baytown, Texas.

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

Kara Bren, Rich Eisenberg, and Bill Jones at the ACS Meeting in San Diego, March 2012

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 Naciónal Autonomas de México.

Bill has also been invited back to China this fall to speak at two meetings, both in Beijing. He will serve on the International Advisory Board for the ICOMC and the ICOM&Cat conferences. The group is supported by continuing funding from the Department of Energy, the National Science Foundation, and the NSF Center Enabling New Technologies through Catalysis. We are just initiating new work with GE on liquid fuel cells.

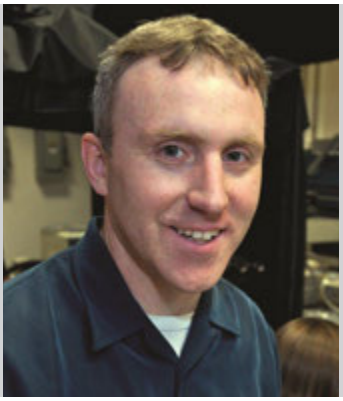


Computer Studies Building

Todd D. Krauss

Professor of Chemistry

Ph.D. 1998, Cornell University



RESEARCH INTERESTS

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

CONTACT

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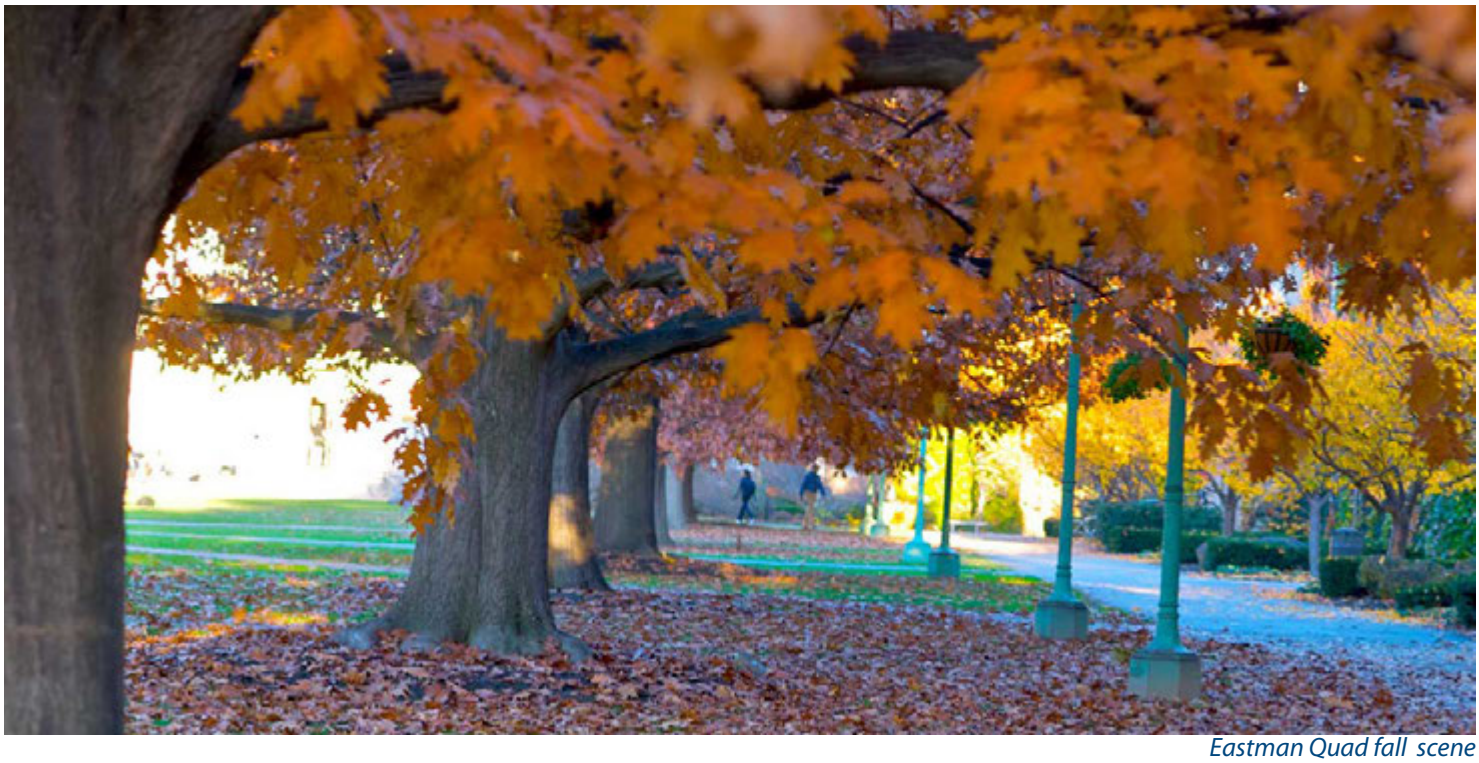
Yet another year of scientific discovery just seems to have flown by for the **TODD KRAUSS** group.

ANDREA LEE (POSTDOC '12) and **WESLEY ASHER (PH.D. '12)**, both co-advised by Prof. Kara Bren, left the group in the last year after working 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 expect they will receive a lot of attention from the community, since they imply single molecule methods may be absolutely necessary to capture the richness of protein structure heterogeneity as it unfolds. Special congratulations to Wes who earned his Ph.D. in May and is now at Columbia University as a postdoctoral research fellow, and to Andrea, who is now in a technical scientist position at the University of Vermont. We wish them both the best of luck in their new positions!

Julie Smyder is finishing up the final drafts of her thesis and has already secured a postdoctoral research fellow position at Cornell University with UR alum John Marohn. Congratulations Julie! Julie is excited about the new position which she hopes to begin (after her PhD. Defense) in the early fall. Jack Calcines is still working on pushing out final thesis chapters on the role of secondary phosphines in the growth properties of semiconductor quantum rods. Helen Wei worked extra hard this past year as she gave birth to baby Emma in May. Congratulations Helen! Helen's paper on growth of quantum dots with controllable surface chemistry using secondary phosphine precursors got excellent reviews in *Nano Letters* and we expect it will be accepted for publication shortly. Like Julie, Helen is also working on writing up her thesis and hopes to defend this year.

Working with Zhiji Hahn, who is co-advised by 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. Zhiji and Fen recently had a tremendous breakthrough, as they were able to produce hydrogen for over two weeks, when common photo-sensitizers last only a day or so. Brad Loesch is close to having enough data to write a new manuscript on using ultrafast optical spectroscopy to explore the process of generating more than one electron per absorbed photon in carbon nanotubes. Lenore Kubie is another one of the Krauss-Bren students and she is working on the photoinduced charge transport between heme containing proteins and carbon nanotubes. Lenore had an exciting summer as she spent four weeks in Ghana learning about the need for inexpensive, distributed and renewable energy firsthand! Finally, Greg Pilgrim and **ANNI SIITONEN**

Lenore Kubie in Ghana



Eastman Quad fall scene

(POSTDOC '12) have been successful fabricating vertically aligned carbon nanotube membranes, which will be used for the production of chemical fuels by sunlight. Initial tests of the membrane show that it can conduct both protons and electrons, which is a rather unique property in any material, and may have several applications. Greg is working on final characterization of the membrane and is preparing to ask the University to file a patent on the invention. Anni left Rochester in the winter and is now in Boston interviewing for technical positions in industry. Good luck Anni!

Nicole Briglio spent much of the past year fighting with the infamous Krauss group IR PMT. To her great credit – she got it working and is on the cusp of getting single carbon nanotube fluorescence measurements at ultracold temperatures (10 Kelvin), which will be quite an accomplishment! Kelly Sowers is working on shelling CdSe quantum dots with CdS and ZnS but using secondary phosphine sulfide precursors. Kelly can now control precisely the amount and chemical composition of the shell on the quantum dots, which should lead to quantum dots with well-controlled optical properties. Cunming Liu is still our first and only materials science student who has been very busy studying the excited state dynamics of CdSe quantum dots and is close to understanding how the excited states of the quantum dot behave under high intensity illumination. Amanda Preske is the NSF-IGERT Fellow in the group and as part of her fellowship she spent 10 weeks at the National Renewable Energy Laboratory as an intern learning how to make PbSe quantum rod solar cells. When she returns Amanda will be working on novel solar cell designs made from quantum dots.

Postdoctoral fellow Dr. Michael Odoi has gotten involved in several projects in the lab. His most recent endeavor is to measure the "spooky" quantum mechanical nature of the photons emitted from single carbon nanotubes, which will tell us how much nanotubes (that by the way can be over several microns long) resemble a single molecule. Dr. Sebastian Schäfer is a new postdoctoral fellow and has gotten off to a great start. He has set up a single molecule electrochemistry apparatus and is busy looking at how applied electrochemical potential affects the fluorescence of individual nanotubes. Zhentao Hou is our newest student and is just getting started with her research on carbon nanotube photophysics.

During the summer the group hosted undergraduates Ian Pershing and Joanne Ledbetter from the University of Rochester. They liked their summer experience so much that they will join another UR undergraduate, Taylor Moot, to complete their senior thesis research with the group this academic year.

Todd is still in the throes of getting a new company started. 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. UR alum **BRETT SWARTZ (M.S. '06, PH.D. '10)** has done an outstanding job of putting the basic ideas behind the company into practice; we are especially excited about the over 5 grams of PbSe quantum dots that Brett made recently.

Finally, Todd adopted a 10-week-old Labrador puppy, named Jeter, in April. The entire group (especially Nicole) is enjoying watching the pup grow and he has quite a following on campus.

Robert W. Kreilick

Professor Emeritus of Chemistry — Ph.D. 1964, Washington University

RESEARCH INTERESTS

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

CONTACT

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ROBERT KREILICK is enjoying his fifth 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. 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 continues his focus on support of graduate and undergraduate education. As chair of the graduate studies committee Tom enjoys working with graduate students. Tom also spends countless hours advising undergraduates in his role on the undergraduate studies committee, especially in terms of fostering undergraduate research. The National Science Foundation renewed our Research Experience for Undergraduates grant, and we had 30 REU participants in summer 2012, including 20 University of Rochester students. A number of our REU participants will be presenting their research at the Northeast Regional ACS Meeting this fall. Tom also served as the elected chair of the Faculty Council Steering Committee this past year.

Entrance to Hutchison Hall

David W. McCamant

Associate Professor of Chemistry

Ph.D. 2004, University of California, Berkeley

RESEARCH INTERESTS

Ultrafast vibrational spectroscopy of structural dynamics in photochemistry; vibrational coupling and relaxation; structural rearrangements in photoinduced charge-transfer molecules and photoexcited nucleic acids.

CONTACT

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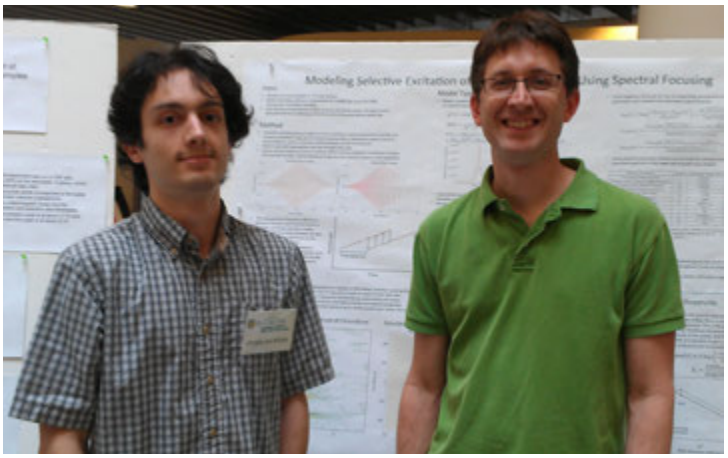
The 2011-2012 year was exciting in the McCamant Lab. **DAVE MCCAMANT** was awarded tenure and so is now "Associate Professor of Chemistry"- a very exciting new title. **JUSTIN RHINEHART (PH.D. '12)** became our first Ph.D. graduate, successfully defending his thesis in December 2011. He's since moved on to a postdoc with Jenny Lockard at Rutgers, Newark. By all accounts, he's doing great there building up some interesting new ultrafast laser experiments. The rest of our entourage included postdoc, Dr. J. Reddy Challa, graduate students Kristina Wilson, Barbara Dunlap, Randy Sabatini, and Joohyun Lee as well as undergraduate **PETER RICHTER (B.S. '12).** Peter is attending MIT this fall, after finishing up his exciting theoretical investigations in our lab of stimulated Raman spectroscopy using chirped picosecond pulses. This work, along with the interesting experiments that test this methodology, performed by Barbara, will be submitted for publication this fall.



Peter Richter and Dave McCamant at the Senior Thesis Poster Session 2012

In technical news, this year saw a cool new thingamajig built on our table; we now have an SHBC ("Second harmonic bandwidth compressor") built by Joohyun, as well as a Hydrogen Raman shifter, which together give us picosecond pulses throughout the UV and visible spectral regions. Reddy and Joohyun have used this system to collect our first transient stimulated Raman signals of dGMP, an important DNA monomer. These new wavelengths allowed interesting work over the summer by Rachel Kozlowski (REU from Campbell Unversity) investigating the ultrafast dynamics of hemes and Joe Colaruotolo, (UR BS '13) who used the UV wavelengths to study the amino acid tryptophan. Overall, it has been a great year for ultrafast laser spectroscopy!

Eastman Theatre

John S. Muenter

Professor Emeritus of Chemistry — Ph.D. 1965, Stanford University

RESEARCH INTERESTS

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

CONTACT

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For **JOHN MUENTER,** the past year has been busy with non-academic interests, but molecular spectroscopy still occupies some of his time. John is continuing to spend one week every couple of months working at MIT with Bob Field's group and in October he was at Oxford University working with Brian Howard. This was the last opportunity for Brian and John to work together as Brian is also retiring, so this trip concluded a very productive collaboration that has been going on for 30 years.

John's week in Oxford lead to the continuation of this project with Mark Marshall and Helen Leung at Amherst College. Brian gave a paper on this work at the Ohio State Molecular Spectroscopy this summer that had authors from Amherst, Oxford and Rochester; a nice recognition of two long collaborations.

Michael Neidig

Assistant Professor of Chemistry — Ph.D. 2007, Stanford University

RESEARCH INTERESTS

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

CONTACT

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MICHAEL NEIDIG'S group has had a busy and exciting first year at Rochester. Our laboratory renovations were completed in January of 2012 and we quickly occupied our new home and got to work on setting up our spectroscopic and synthetic capabilities, including our magnetic circular dichroism instrument. We have spent the remainder of 2012 moving forward with our research on iron catalysis in organometallic chemistry and for small molecule activation. Our group size has grown over the past year with the addition of three first year Ph.D. students: Stephanie Daifuku, James Virnelli and Jared Kneebone. We were excited to have **BEN SNYDER (B.S. '12)** with us from January, following his completion of the B.S. chemistry degree, until the end of June. He has now moved on to pursue a Ph.D. in chemistry at Stanford University. We have also had three additional students in the group this summer: Chris Valente, a summer REU student from Bucknell University, and two new Ph.D. students starting in the program this fall, Katy Fillman and Katryna Pellingra. Next year promises to build upon our initial research momentum and we look forward to continuing our work on iron catalysis.

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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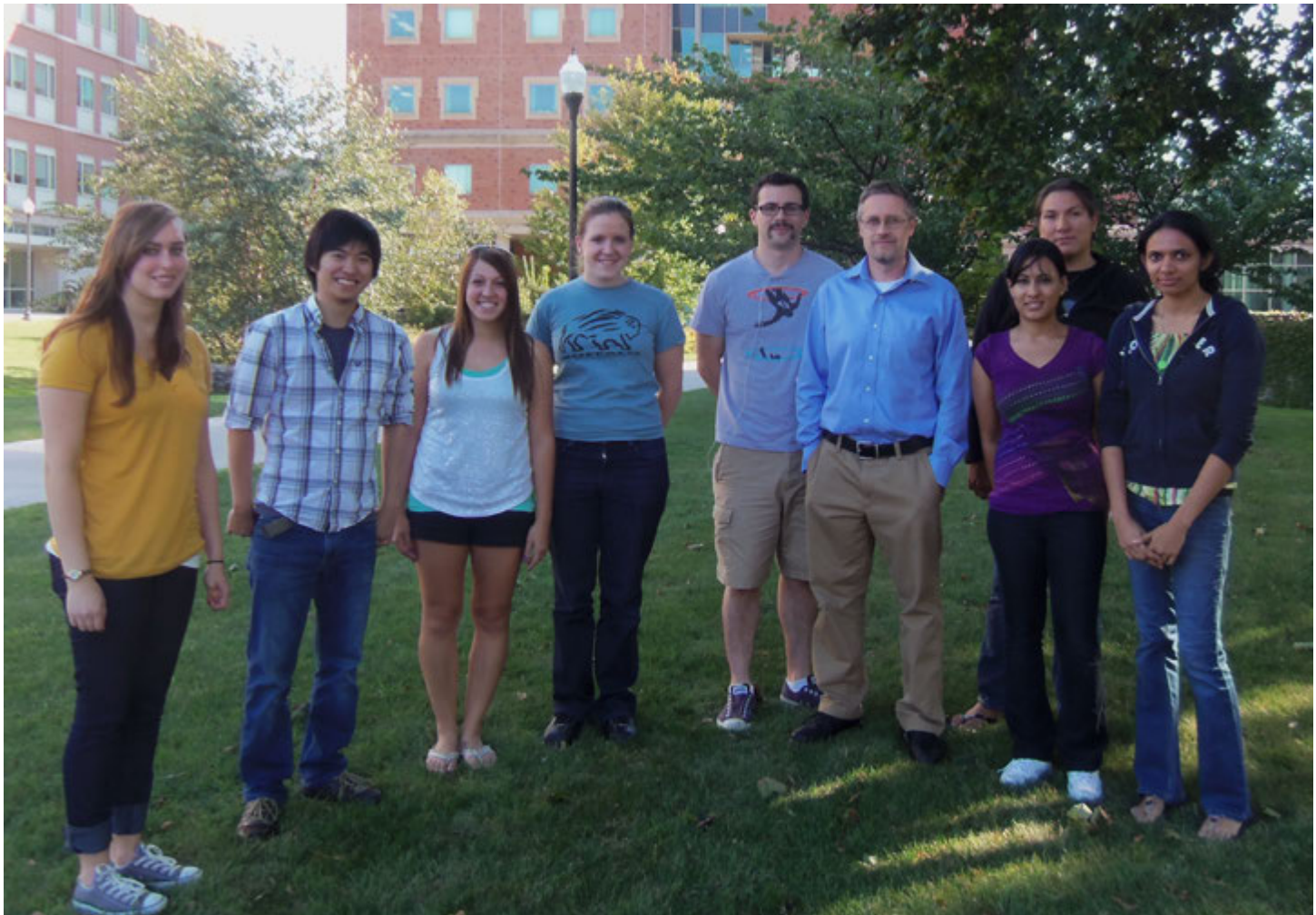
The **BRAD NILSSO**N group has experienced some dramatic changes in the last year. Our research efforts have continued to expand while the complexion of the group has changed. The past 18 months have seen four graduate students successfully finish their Ph.D. studies, including two in the last 12 months. **CHARLES BOWERMAN (PH.D. '11)** defended his Ph.D. thesis (October 2011) and subsequently moved to a postdoctoral position with Professor Joseph DeSimone (University of North Carolina). Charlie's research in the DeSimone lab involves the creation of materials for biomedical applications. He has excelled in the DeSimone group and within several months of starting his postdoctoral appointment he was promoted to a research scientist position. This appointment is for 3 years and gives him supervisory and grant-writing responsibilities over the oncology efforts in the DeSimone lab. **TODD DORAN (PH.D. '11)** also completed his Ph.D. studies (December 2011) and is a postdoctoral research fellow with Professor Tom Kodadek at Scripps Research Institute, Florida. Todd is engaged in efforts to design new therapies for diabetes and associated disorders. We congratulate Charlie and Todd on their success this past year. With the previous departures of **DEREK RYAN (PH.D. '11)** and **TIMUR SENGUEN (PH.D. '11)** the personality of the group has evolved.

Naomi Lee is nearing the end of her graduate studies. She will defend her Ph.D. thesis in October 2012 and will then



move to a postdoctoral position at the National Institutes of Health in Bethesda, MD. She is in the final stages of manuscript/thesis preparation for each of her projects. Collectively, Naomi's work has contributed to significant insight into the self-assembly of short, amphipathic peptides into amyloid-like fibrils and is enabling work in our group that seeks to exploit these peptides as novel bioactive materials.

John DiMaio and Ria Swanekamp are entering their fifth year of graduate study and, along with Naomi, have assumed the mantle of seniority in the group. John continues his research on the role of naturally occurring amyloid in HIV transmission processes (*J. Biol. Chem.* **2012**, *287*, 11842–11849); he is also developing novel amyloid-inspired materials that will function as microbicides for the prevention of the sexual transmission of HIV in collaboration with Steve Dewhurst's group (University of Rochester Medical Center, Department of Microbiology and Immunology). Ria is involved in several projects as well. She has recently reported the unexpected co-assembly of enantiomeric peptides into two-component hybrid fibrils (*J. Am. Chem. Soc.* **2012**, *134*, 5556–5559). This work was featured in a "Spotlights on Recent JACS Publications" article (*J. Am. Chem. Soc.* **2012**, *134*, 6057); she also presented this work at a recent Chemistry and Biology of Peptides Gordon Conference and Research Symposium. Ria is also involved in a new project in the Nilsson group focused on the use of amphipathic peptides as novel delivery agents for therapeutic oligonucleotides.

Wathsala Liyanage and Annanda Rajbhandary are engaged in efforts to develop amino acid-based self-assembling hydrogel materials for tissue engineering applications. This work has been funded by a recent CAREER Award from the National Science Foundation ("CAREER: Amyloid-Inspired Self-Assembled Hydrogel Materials for Cell Culture Applications", DMR-1148836). Both Wathsala and Annada have made tremendous progress on this work in the last year; Wathsala received a Travel Award from the American Chemical Society to present her work at the National ACS Meeting in Philadelphia this summer.

Our talented group of undergraduate research students has also met with great success in the last year. **SAM ANDERSON (B.S. '11)**, who conducted his senior thesis research in the Nilsson lab in the 2010-2011 academic year has recently been awarded an NSF predoctoral fellowship in support of his graduate work in chemistry at the University of North Carolina. We congratulate Sam on this great accomplishment! **REBECCA LEVIN (B.S. '12)** and **EMILY HART (B.S. '12)** each completed their senior research in the Nilsson group this last year. Rebecca is attending medical school at Boston University and Emily has moved to New York City to teach high school science as part of the Teach for America program. Both Rebecca and Emily were outstanding students that made significant contributions to projects that are currently being prepared for publication in peer-reviewed journals. We wish them success in their future endeavors. Several new undergraduate students have joined the lab in the last year. Annah Moore (a rising sophomore) has worked in the lab over the summer on our HIV microbicide project and Genki Tamiya (a rising senior) will conduct senior research in the Nilsson group this year.

Our research efforts have been fruitful in the last year as well. In addition to the work highlighted above, we have also published other significant articles in the last year. We have reported the results of our efforts to understand the role of turn formation in the self-assembly of the Alzheimer's disease amyloid-b peptide (*ACS Chem. Neurosci.* **2012**, *3*, 211–220; *J. Mol. Biol.* **2012**, *421*, 315–328). These studies shed light on the nature of turn nucleation in amyloid self-assembly processes and also provide insight into novel strategies to perturb amyloid self-assembly. We have published additional work regarding the role of aromatic effects on amyloid self-assembly (*Proteins* **2012**, *80*, 1053–1065; *Biopolymers* **2012**, *98*, 165–184) and have also reported new advances in our efforts to create amyloid-inspired hydrogel materials *(Langmuir* **2012**, *27,* 11145–11156; *Polym. Chem.* **2012**, *3*, 18–33). We are excited about the momentum we've built in these areas and look forward to expanded efforts in these and new research directions in the coming year.

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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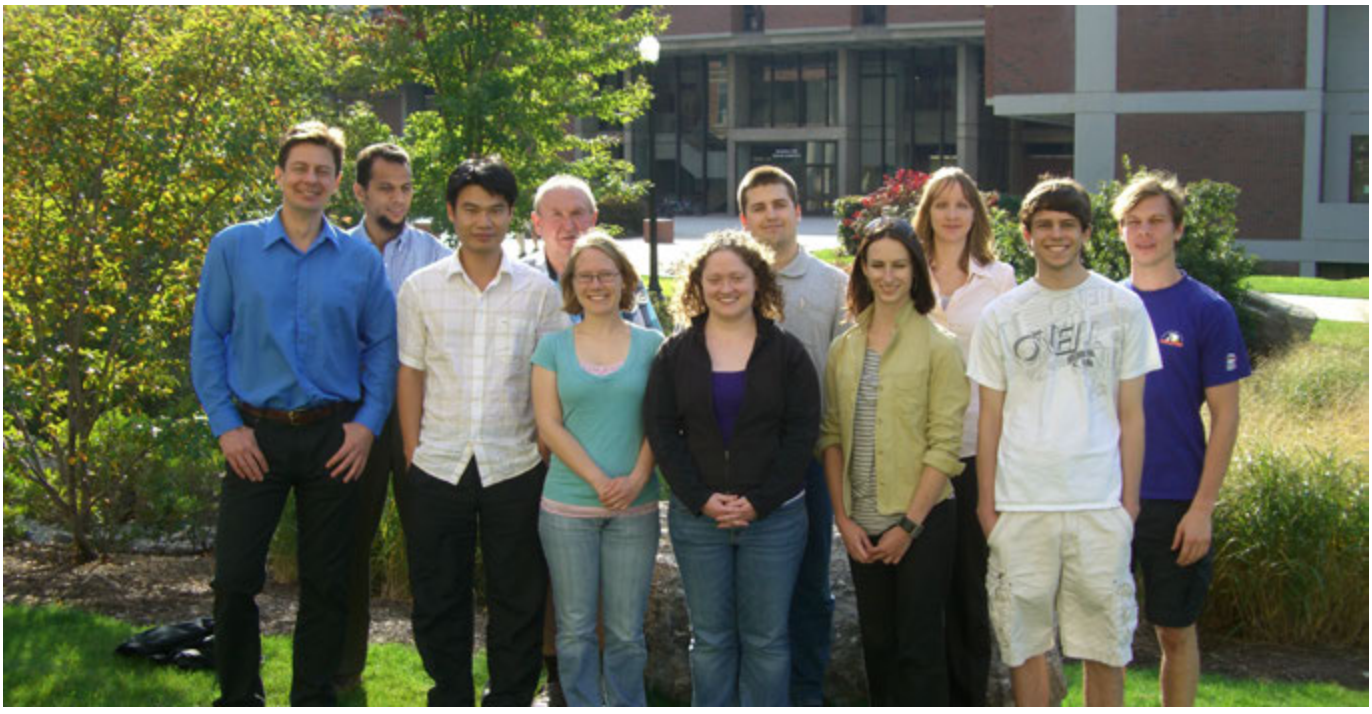
The **OLEG PREZHDO** group has grown to its "steady-state" size of about ten people. Several group members have found academic positions: **VITALI CHABAN (POSTDOC '12)** will be a Group Leader in the Center for BioMembrane Physics at the University of Southern Denmark; **RUN LONG (POSTDOC '12)** has become a Lecturer at the University College Dublin in Ireland; **KIRILL IGUMENCHSHEV (PH.D. '11)** is a Postdoc at UC-Berkeley with Bill Miller. Dr. Alexey Akimov, Ph.D., from Rice University has joined the group. Ahmed Mustafa is staying with the group on a visiting scientist fellowship from Egypt. A recipient of a European Union exchange grant, Igor Vovchinskyi from Kharkov, Ukraine will arrive within the next few months. Several group members spent their summer in national labs, gaining valuable research experience in premier scientific environments. Olena Postupna and Tammie Nelson worked with Dr. Sergei Tretiak in the Los Alamos National Lab. Alexey Akimov collaborates with Jim Muckerman in Brookhaven National Lab. Amanda Neukirch is implementing the theoretical developed in the Prezhdo group within a code developed by James Lewis in West Virginia University.

Over the last year, Oleg Prezhdo and his group members presented a couple dozen invited talks, published over 30 papers, including a book chapter, 4 reviews, 4 editorials, and 29 regular articles. The work by Vitaly Chaban published in ACS Nano in 2011 and 2012 was highlighted in the New Scientist magazine, in public news, and on multiple web-pages around the world. The paper by Run Long was chosen for the *Journal of the American Chemical Society Spotlights*.

Oleg Prezhdo organized a symposium in the March 2012 ACS Conference, an International Workshop in the Tellu-



The Prezhdo Group

ride Science Center, and a symposium at the SPIE optical society meeting. He edited a special issue in Surface Science, devoted to graphene. His DOE grant was renewed, and he was awarded part of the joined DOE grant initiated by the Brookhaven Lab. Oleg Prezhdo became an Invited Professor at the Université Paris Est, France, and was awarded the Promising Scientist Prize of CMOA (Centre de Mécanique Ondulatoire Appliquée).

In 2011, Oleg 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. Just published, its impact factor is 6.2. The *Letters* is proud to report a very fast time from submission to web publication of only 40 days, compared to the 70-90 days typical of the majority of journals. Oleg's wife Marina is helping Oleg to handle the journal duties.

On a personal note, Marina co-founded the Russian Sunday School "Sunshine" for children aimed at maintaining the Russian culture and teaching the children the Russian language, history and arts. Marina's & Oleg's older daughter Eugenia (21) 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. In 2012, she graduated Magna Cum Laude from the University of Rochester with a major in Mathematics and a minor in Brain and Cognitive Science. Eugenia's first paper was published in the *Biophysical Journal.* Their younger daughter Natalie (8) has finished the 2nd grade in the Mendon Center Elementary school in Pittsford. She is a regular in the Rochester Chess Club and studies ballet in the Timothy M. Draper center for Dance Education.

Lewis J. Rothberg

Professor of Chemistry

Ph.D. 1983, Harvard University

RESEARCH INTERESTS

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

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LEWIS ROTHBERG'S group continues its research at the frontiers of organic electronics and plasmonics. We work closely with the Tang and Chen groups on applications including improved light extraction from organic light-emitting diodes (OLEDs), development of host materials for blue phosphors and improvement of thin-film photovoltaics. Alex Shveyd and Austin He have begun pioneering studies of degradation in blue OLEDs using time-of-flight mass spectrometry to analyze degradation chemistry in devices and we expect their upcoming publications to make a big splash. Chi-Sheng Chang, along with an energetic summer REU student Rebecca Brumbaugh, is working with the Tang group and eMagin Corporation to make efficient scattering layers using silver nanoparticles to improve OLED efficiency. Their work is soon to be matched up with theory being done by a new postdoctoral student, Irfan, and Chemical Engineering MS student Guy Mongelli. We are very excited that we will see the first results integrating these with OLED technology in a few months. Working closely with the Tang group has been great and helps to connect our work into the mainstream of organic electronics! It's amazing to reflect on how far our field has come, highlighted by achievements like the recent introduction of 55 inch diagonal televisions based on OLED technology. Lewis has also been privileged to work closely with Tang's students including Guy Mongelli mentioned above, Hui Wang (modeling of OLEDs) and Sangmin Lee (whose paper was selected as one of the distinguished papers of the Society for Information and Display conference in 2012).

At the same time, we are pursuing fundamental research on organic chromophore photophysics including suppression of photodegradation (Steve Paquette), studies of blue phosphors (Kelly Sassin), interpretation of delayed photoluminescence (Millard Wyman and new student Rajarshi Chakraborty),

The Rothberg Group

excited state dynamics in model conjugated polymers (Zanny Stwertka), properties of interlayers in tandem organic solar cells (Chris Favaro) and spectroscopy of single polymer chains (Ben Martin). Xiao Wang and UR undergraduate Greg McKay are working with colleagues from the Cornell Agriculture School to apply reflective interferometry to stone fruit pathogen detection under funding from the University to develop data to help commercialize the technology and intellectual property we have generated.

Always a source of fun and stimulation is our work with undergraduate researchers. Aside from Greg and Rebecca mentioned above, **JONATHAN RAYBIN (B.S. '12)** (solvent dependence of polythiophene spectroscopy), **CINDY WU (B.S. '12)** (DNA adsorption on surfaces) and Susan Pratt from Physics (variations of reflective interferometry) were seniors who worked with Lewis and are now off to prestigious graduate institutions. We are also blessed with funding from the NSF to support Thomas Bertrand, a teacher from Webster High School, for two summers to develop and disseminate learning modules for secondary schools that leverage the excitement of the organic electronics research. Lewis is thankful too for the important contributions of a number of active senior scientists affiliated with the group including William Begley, Al Marchetti, Barbara Stwertka and Ralph Young who not only do excellent science but also contribute mightily to the mentorship of students.

Lewis took new energy into teaching general chemistry (CHM 132) and participated actively in the workshop program led this year by our alumnus **NIC HAMMOND (PH.D. '11)**. It was great to be working with Nic, Jim Farrar and Ben Hafensteiner on the course and we can be proud of the educational product. Lewis also taught the advanced spectroscopy lab (CHM 232) with able assistance from **RAY TENG (B.S. '83, M.S. '87, M.B.A. '01)** and Ben Martin in addition to a fine cadre of teaching fellows. Other notable events around campus include the departure of valued collaborator and colleague Philippe Fauchet and the unfortunate death of our respected and enthusiastic colleague Bill Bernhard. We also celebrated mother and Professor of Chemistry Esther Conwell's 90th birthday and continue to marvel at her continued interest in and facility for scientific research.

Lewis presented work at many meetings and institutional seminars. The most memorable conference was the OP2011 conference in Santa Fe which is the tenth in a vital and growing series started by Valy Vardeny and Lewis in 1994. The most gratifying colloquium visit was at the University of Alabama where former graduate student **PROF. SHANLIN PAN (PH.D. '06)** is doing extremely well and enjoying a highly productive and innovative pre-tenure period. Lewis was also interviewed on a blog sponsored by Nature Chemistry where he had the fun of choosing books to take to a desert island and imagining alternative careers. The web link can be found at http://blogs.nature.com/thescepticalchymist/2012/06/reactions-lewis-rothberg.html#wpn-more-3769.

Diffinity Genomics, a company spun out of the group's research, continue to rent R&D space in Hutchison and manufacture product in Henrietta. They introduced a second product for PCR purification prior to enzymatic reactions that precede cloning and are on a trajectory to expand and move to other space in the next couple of years. It's been an exciting and educational experience and the exposure of the students to small company life and the outstanding people who work for the company has been a valuable added dimension to working in the group.

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.

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For **WILLIAM SAUNDERS,** the summer of 2011 began with a trip to Germany for biking and barging. Bill spent three days in Berlin at the beginning, a fascinating combination of the old, new, and avant garde. There followed a trip by barge along the Mosel River, finishing in Luxembourg. They rode bikes during the day and ate and slept on the barge at night. August 25-27 he spent in Stratford, Ontario seeing plays at the Shakespeare Festival, including The Misanthrope (Moliere), Richard III (Shakespeare), and The Homecoming (Pinter). This year the family came to Rochester for Thanksgiving rather than Christmas. At Christmas time Bill went to visit Anne and the granddaughters in New Hampshire, followed by a day in Boston before returning home. In February Bill attended the Gordon Isotopes Conference. Around the same time he became a bionic man by having a cataract operation in which the dimming lenses of his eyes were replaced by plastic substitutes, much improving his vision. The spring as well as the early summer have been unusually warm – perhaps a warning of global warming. Bill continues calculations on product proportions in elimination reactions in collaboration with a colleague at Virginia Commonwealth University, Scott Gronert.

Bausch and Lomb

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.

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UDO SCHRÖDER'S group continued research in radiochemistry, heavy-ion reaction dynamics, their new nuclear plasma physics research program, and in technical R&D.

Experimental and theoretical results on the disintegration of hot nuclear systems produced in heavy-ion induced reactions have been presented by several group members at national and international conferences. Theoretical investigations of nuclear instabilities, conducted in the framework of an interacting Fermi gas model and leading to the discovery of surface boiling, a new nuclear decay mechanism, have been reported by Jan Tõke at the IWMF 2011 multifragmentation meeting in Caen and the Nucleus-Nucleus 2012 Conference. This area remains an important research focus by the group, addressing next specific associated isospin fractionation effects. Results obtained from the experimental research program conducted by the group in collaboration with Italian groups at the LNS Catania laboratory, demonstrating "isoscaling" regularities in the isotopic distributions from non-statistical projectile breakup following dissipative interactions, have also been reported (by Udo) at the IWMF 2011. The group's new ASTERICS silicon-strip detector has undergone first in-beam tests. Our graduate students Sheth Nyibule and Eric Henry have spent part of summer with these tests at LNS (see Figs. 1 and 2). Sheth is the proud recipient of a travel and research grant from the Italian funding agency INFN.

On his research stay at LNS Catania this summer, UR student Sheth Nyibule (right) is working with LNS nuclear scientist Luis Acosta (left) at a small LNS Catania detector test stand.

Radio-chemical research into tritium transport has made good progress, as grad student **MATT SHARPE (B.S. '09, M.S. '11)** has solved some technical problems with his plasma induced sputtering experiment. The group's new research proposal to explore laser induced ion acceleration (and reactions) for nuclear experiments (LIANE) has been accepted and measurements are under preparation for isotopically enriched Li-compound targets.

Congrats are due to former graduate student **MIKE QUINLAN (PH.D. '12)**, who defended his Ph.D. thesis last year, as well as to Ben Hmiel and Matt Goodman, who both received M.S. degrees. Mike now works at the Lawrence Berkeley National Lab, location of our, now ancient, pioneering heavy-ion experiments. Ben is hoping to apply his nuclear technology expertise in Antarctic paleoclimatology as a geology grad student. Matt is still finishing up an LLE project and intends to leave grad school in pursuit of a practical laboratory career.

The Advanced Nuclear Science Education Laboratory (ANSEL), run jointly with the Department of Physics and Astronomy, continues to thrive. Creation of this lab was funded by an NRC grant and enabled by the commitment and strong support by Chemistry and Physics Depart-

ments, as well as by the UR Medical Center and the Laboratory for Laser Energetics. In addition to teaching the ANSEL, Udo has given a series of lectures in the Nuclear Chemistry Summer School 2012 held by the American Chemical Society at Brookhaven National Laboratory.

UR's Sheth (right) with Luis (left) checking setup with the LNS CHIMERA multi-detector array.

Harry A. Stern

Assistant Professor of Chemistry

Ph.D. 2001, Columbia University

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 has left the chemistry department for greener pastures and is now working with the Center for Integrated Research Computing (CIRC) here at UR. Don't ask him what the "integrated" means; it is all about the acronym. In his new position he is working with research groups across campus on calculations and simulations, assisting with maintaining the Center's extensive computational resources, and writing grants (that never ends). Harry has moved all of 100 yards down Hutchison Road and encourages anyone doing computational chemistry to get in touch with him with any questions, or just to visit lovely Taylor Hall. Former graduate students **CEN GAO (PH.D. '09)** and **MIN-SUN PARK (PH.D. '11)** are both doing well. Cen is a computational chemist at Eli Lilly in Indianapolis, and Min-Sun is a postdoc in Tamir Gonen's lab at the HHMI Janelia Farm Research Campus in Virginia.

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.

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This year, the **DOUG TURNER** group made progress on "getting" the flu. Several years ago, the group started working on influenza A as part of a long term goal to develop a pipeline from genomic sequences to therapeutics. The genome of influenza is made of about 10,000 nucleotides of RNA that are contained in eight separate segments that range from roughly 850 to 2500 nucleotides. In 2011, **WALTER MOSS (PH.D. '11)** and Sal Priore published predictions of secondary structures for five short regions of influenza messenger RNA. Upon receiving his Ph.D., Walter remained in the lab to team with his wife, Indee Dela-Moss, Sal, and Ryszard and **ELA KIERZEK (POSTDOC '03-05)** to test a structural prediction for a splice site that controls the relative production of two essential proteins, M1 and M2. They discovered that the sequence can fold into two different conformations, one that likely allows RNA splicing resulting in M2 and the other inhibiting splicing so that M1 is produced. **JON CHEN (OPTICS B.S. '06)** and Andy Kauffmann have started NMR studies to determine the 3D structures of this RNA switch. Sal, Tian Jiang, and undergraduate, Jayson Baman, are testing predictions for other regions. The NMR studies are being done in collaboration with Scott Kennedy from the Department of Biochemistry and Biophysics. So, construction of the pipeline is off to an exciting start. The hope is that the end of the pipeline will include collaborations with the Kierzeks and with **MATT DISNEY (PH.D. '02)** to discover therapeutics that inhibit influenza.

Walter and Sal also used free energy minimization programs to predict which influenza segments are likely on average to have significant amounts of structure, which they call "Global Ordered RNA Structure," abbreviated as GORS. Four of the eight segments have messenger RNAs that exhibit this trend, but none of the genomic RNAs have GORS. The results have implications for design of live vaccines. Differences in predictions for messenger and genomic RNAs depend on the thermodynamics for GU and CA pairs because a GU pair in the folding of a messenger RNA becomes a CA pair in the complementary genomic RNA, and vice versa. To make better predictions of GU pairs, Jon Chen in collaboration with Marty Serra from Allegheny College expanded the database of thermodynamics for duplexes containing GU pairs and published revised nearest neighbor parameters for inclusion in prediction algorithms.

The group also continued to help develop methods for predicting 3D structures of RNA. In collaboration with Scott Kennedy, Harry Stern, Ryszard Kierzek, and **JIM HART (PH.D. '08), ILYAS YILDIRIM (PHYSICS PH.D. '08)** published a paper showing that his revisions of parameters in the AMBER force field improve predictions of relative equilibrium constants for tetramer duplexes by up to 10 orders of magnitude. Doug helped **DAVE MATHEWS (PH.D. '01)** think about computational results aimed at understanding an internal loop conformational switch previously published by **GANG CHEN (PH.D. '05). NIC HAMMOND (PH.D. '11)** returned from a two year teaching position at Boston University and defended his thesis before taking a position as Assistant Director of UR's Workshop Program. An internal loop that Nic described in his Biochemistry paper published in 2010 is receiving recognition as a novel structure useful as a benchmark for testing algorithms that predict 3D structure.

Doug enjoyed attending three meetings: an RNA Dynamics meeting in Telluride where he, Dave Mathews, and **PHIL BEVILAQUA (PH.D. '93)** gave talks, an ACS meeting in San Diego where he gave a "warm up" talk preceding Matt Disney's talk accepting the New Investigator Award of the Carbohydrate Division, and the third annual UR Chemistry-Biology-Biophysics Interface Retreat, which he organized with Terri Clark and which is described elsewhere in this Newsletter.

Outdoor stairs to the plaza

The Rochester weather has apparently encouraged several group members to reside in the south. This started with **DIANE BATES (PH.D. '81)** joining Abbott Labs in Dallas in the 80's. This year, **TIANBING XIA (PH.D. '99)** joined Jim Hart at Abbott in Dallas, and **JAMES KIM (M.D./PH.D. '97)** became an Assistant Professor at the University of Texas Southwestern Medical Center at Dallas. **SUSAN SCHROEDER (PH.D. '02)** was promoted to Associate Professor with tenure at the University of Oklahoma. **BLANTON TOLBERT (PH.D. '06)** countered the trend by moving his lab from Miami University in southern Ohio to Case Western University in Cleveland.

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 made large strides in our understanding of how to go about making C-C bonds through the combination of two different electrophiles instead of the usual electrophile + nucleophile. Through mechanistic studies by Ruja Shrestha, Daniel Everson, and Dr. Soumik Biswas, we now have a good idea of why successful reactions succeed and why unsuccessful reactions fail. These results will be published shortly. In the meantime, the group is busy applying this understanding to the development of new and better reactions. Alex's paper on the synthesis of ketones from carboxylic acid derivatives and alkyl halides was published, as was Dan Everson's full paper on the coupling of aryl bromides with alkyl bromides. Dan Everson and **BRITTANY JONE'S (BS '11)** manuscript was highlighted in Chemistry World.

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Finally, it seems that everyone in the group is working on a paper at the moment, so we look forward to a busy 2012/2013.

In group news, we welcomed two new graduate students this year: Jill Caputo and Yang Zhao. In addition, we welcomed a new undergraduate researcher, Ryan Ribson ('14). The group now has 10 full-time researchers plus four active undergraduates. **RUJA SHRESTHA (PH.D. 2012)** defended her thesis in April, and moved on to a postdoctoral position with Prof. John F. Hartwig at the University of California, Berkeley. We miss her already! Alex Wotal passed his oral exam and is tackling his research full-time now. **ADAM LEE (B.A. '12)** graduated and is attending medical school this fall back home at the University of the West Indies (Jamaica).

Once again, several group members have been recognized for their efforts in the lab and the classroom this past year. Jill Caputo and Stephanie Dorn were awarded W.D. Walters teaching awards by the department and Ruja Shrestha was awarded a Elon Huntington Hooker fellowship. Rachel Kelemen ('13) won the College Writing Colloquium contest in the natural sciences category for her paper on "New Advances in Selective, Versatile Carbon-Carbon Bond Formation: Suzuki Coupling with Alkyl Partners" which she wrote for Chemistry 234W lab.

CONGRATULATIONS TO ALL OUR GRADUATES!

Weix Group, Saying Good-bye to Ruja (middle front)

Enjoying S'mores

Publications '11-'12

Includes publications accepted or submitted between July 2011 and June 2012.

ROBERT K. BOECKMAN, JR.

Terpene Derived Auxiliaries: Camphor and Pinene Derived Auxiliaries. J. R. Cody, and R. K. Boeckman Jr., *Synthetic Methods II - Chiral Auxiliaries, Comprehensive Chirality Vol. 3* R. K. Boeckman, Jr., Ed.; Elsevier Science, Oxford UK, **2012;** 1148-1211.

R. K. Boeckman Jr., Ed. *Synthetic Methods II - Chiral Auxilliaries, Comprehensive Chirality Vol. 3*, Elsevier Science, Oxford UK, **2012**.

KARA L. BREN

Comparing Specificity Between Cytochrome *c* Maturation and Cytochrome *c* Heme Lyase Systems for Cytochrome *c* Biogenesis. J. G. Kleingardner and K. L. Bren, *Metallomics,* **2011**, *3*, 396-403.

Temperature Dependent Equilibrium Native to Unfolded Protein Dynamics and Properties Observed with IR Absorption and 2D IR Vibrational Echo Experiments. J. K. Chung, M. C. Thielges, S. E. J. Bowman, K. L. Bren, and M. D. Fayer, *J. Am. Chem. Soc.*, **2011**, *133*, 6681-6691.

Methionine Ligand Lability in Bacterial Monoheme Cytochromes *c*: An Electrochemical Study. B. D. Levin, M. Can, S. E. J. Bowman, K. L. Bren, and S. J. Elliott. *J. Phys. Chem. B*, **2011**, *115*, 11718-11726.

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Heme-Protein Vibrational Couplings in Cytochrome *c* Provide a Dynamic Link that Connects the Heme-Iron and the Protein Surface. M. G. I. Galinato, J. G. Kleingardner, S. E. J. Bowman, E. E. Alp, J. Zhao, K. L. Bren, and N. Lehnert, *Proc. Natl. Acad Sci. U.S.A.*, **2012**, *109*, 8896-8900.

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JOSEPH P. DINNOCENZO

Bimolecular Electron Transfers That Deviate from the Sandros–Boltzmann Dependence on Free Energy: Steric Effect. P. Luo, J. P. Dinnocenzo, P. B. Merkel, R. H. Young, and S. J. Farid, *J. Org. Chem.* **2012,** *77*, 1632-1639.

RICHARD EISENBERG

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Synthesis and Characterization of New Neutral, Luminescent Diphosphine Pyrrole- and Indole-aldimine Copper(I) Complexes. M. G. Crestani, G. F. Manbeck, W. W. Brennessel, T. M. McCormick, and R. Eisenberg, *Inorg. Chem.* **2011**, *50*, 7172-7188.

Non-innocence in Metal Complexes: A Dithiolene Dawn. R. Eisenberg and H. Gray, *Inorg. Chem.,* **2011**, *50*, 9741-9751.

The Impact of Ligand Exchange in Hydrogen Production from Cobaloxime-Fluorescein Photocatalytic Assemblies. T. M. McCormick, Z. Han, D. J. Weinberg, P. L. Holland, and R. Eisenberg, *Inorg. Chem.,* **2011**, *50*, 10660-10666.

A Cobalt-Dithiolene Complex for the Photocatalytic and Electrocatalytic Reduction of Protons. W. R. McNamara, Z. Han, P. J. Alperin, W. W. Brennessel, P. L. Holland, and R. Eisenberg, *J. Am. Chem. Soc.,* **2011**, *133*, 15368-15371.

Trigonal Prismatic Coordination in Tris(dithiolene) Complexes: Guilty or Just Non-innocent? R. Eisenberg, *Coord. Chem. Rev.* **2011**, *255*, 825-836.

A Nickel Thiolate Catalyst for the Long-Lived Photocatalytic Production of Hydrogen in a Noble-Metal-Free System. Z. Han, W. R. McNamara, M.-S. Eum, P. L. Holland, and R. Eisenberg, *Angew. Chem. Int. Ed.*, **2012**, *51*, 1667-1670.

Catalysts Made of Earth-Abundant Elements (Co, Ni, Fe) for Water Splitting: Recent Progress and Future Challenges. P. Du and R. Eisenberg, *Energy Environ. Sci.*, **2012**, *5*, 6012-6021.

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Molecular Systems for Light Driven Hydrogen Production.W. T. Eckenhoff and R. Eisenberg, *Dalton Trans.,* **2012**.

SAMIR FARID

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JAMES M. FARRAR

Imaging Ion-Molecule Reactions: Charge Transfer and C-N Bond-Formation in the $C^+ + NH_3$ system. L. Pei and J. M. Farrar, *J. Chem. Phys.,* **2012,** *136,* 204305.

RUDI FASAN

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WILLIAM D. JONES

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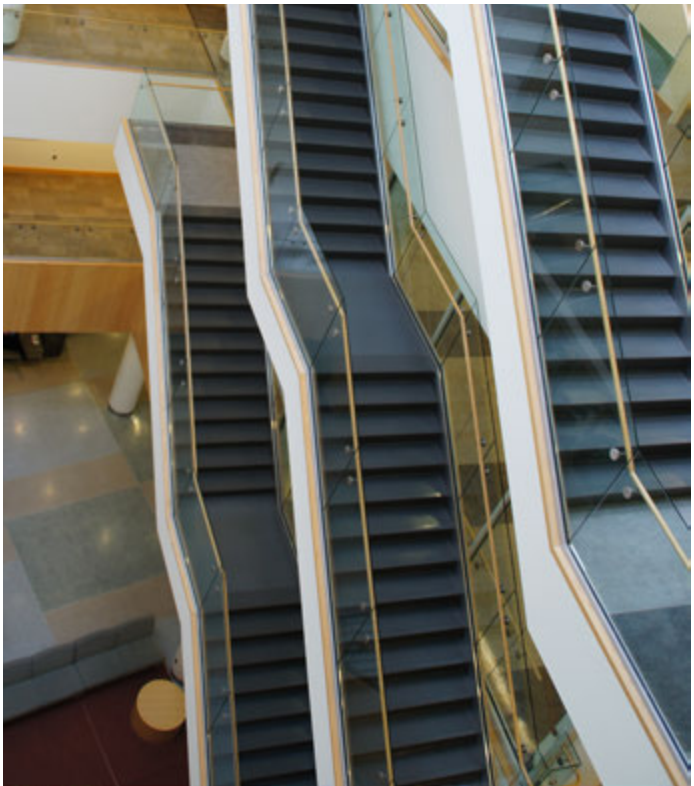
Munnerlyn Atrium, - Goergen



Commencement

Bachelors and Masters Degrees Awarded in Chemistry

2012 BACHELOR OF SCIENCE

Jonathan Goldberg[1]
Emily Hart[2]
Hyun-uk Kang[1]
Ta-Chun Kao
David Kaphan[3†]
Mark Levin[3†]
Rebecca Levin[2†]
Gabrielle Mariano
Jennifer Morey
Jonathan Raybin[3†]
Adbel Reyes
Peter Richter[2†]
Benjamin Snyder[3]
Peter Ting[1]
Cindy Wu
Madeline Yin

2012 MASTER OF SCIENCE

Laura Ackerman
Lukiana Anka-Lufford
Kyle Biegasiewicz
Chi Chen
Matthew Goodman
Benjamin Hmiel
Joshua Kolev
Joohyun Lee
Kimberly Manbeck
Gregory Pilgrim
Amanda Preske
Shaun Shahan
Douglas Tusch
Aaron Walsh
Alexander Wotal
Wenwen Yao

2012 BACHELOR OF ARTS

Kaily Abbott[1]
Benjamin Bovarnick
Jessica Christiano[2]
Jessica Colorado
Matthew DeMars II[3†]
Katherine Garner[2*]
Faye Gura[1]
Soaiful Islam
Katherine Keifer[3†]
Samina Khan[1**]
Daniel Lane*
Adam Lee[2]
Irina Lerman[3]
Alyson Meyer[2]
Maryam Mohammed[3†]
Emma Mrowka
Palida Noor[1]
Christopher Nyiri
Cihangir Okuyan[1]
Emily Redman[3†]
Abdel Reyes
Benjamin Rueda
Allison Shaber
Michael Smith[2]

DISTINCTIONS

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

2012 Chemistry Graduates

Doctoral Degrees Awarded in Chemistry

Wesley Asher
Engineering Native and Artificial Heme c Containing Proteins for Biochemical Applications and Studies of Protein Folding
Kara L. Bren

Charles Bowerman
Insights into the Principles of Amphipathic Peptide Self-Assembly
Bradley Nilsson

Mehmet Can
Factors Affecting the Heme Electronic Structure of Proteins with Heme c
Kara L. Bren

Karen Chiang
Low-coordinate Iron(I) and Iron(II) Compounds as Model Complexes for Nitrogenase
Patrick Holland

Ryan Cowley
Three-Coordinate Iron Complexes with Terminal Imido Ligands
Patrick Holland

Todd Doran
Role of Hydrophobicity, Aromaticity and Turn Nucleation in Peptide Self-Assembly
Bradley Nilsson

Thomas Dugan
A Masked Two-Coordinate Cobalt (I) Complex that Activates C-F Bonds
Patrick Holland

Nicholas Hammond
1. Investigating the Mechanism of Hoechst 33258 Inhibition of Candida spp. Growth and 2. RNA Internal Loops with Tandem AG Pairs
Douglas H. Turner

Kirill Igumenshchev
Quantum Breathers in Dynamics of a Coherent State
Oleg Prezhdo

Sang Min Lee
Organic Light Emitting Devices with Linearly-Graded Mixed Host Architecture
Ching Tang

Mary Lenczewski
Mechanistic Studies of Benzylsilane and Benzylgermane Cation Radicals
Joseph Dinnocenzo

Pu Luo
Mechanism for the Fragmentation of Aryltrialkylstannane Cation Radicals
Joseph Dinnocenzo

Gerald Manbeck
Synthesis and Photoluminescence of Copper(I) Triazole Complexes and Copper(I)/Gold(I) Clusters
Richard Eisenberg

Matthew McLaughlin
Part I. Apo Azurin and its Mutants as Mononuclear Metal Scaffolds; Part II. Homogeneous Photogeneration of Hydrogen from Aqueous Solutions
Patrick Holland

Walter Moss
RNA Secondary Structure Discovery and Characterization
Douglas H. Turner

Jing Qiao
Thermodynamic and NMR Structural Studies of RNA Hairpin Loops
Thomas Krugh

Michael Quinlan
Non-Equilibrium Splits of the Projectile and the Mechanism of Ca + Sn Reactions at 45 AMeV
Udo Schröder

Jennifer Rhinehart
Development of Novel Rhodium and Iridium Complexes with a fac-Chelating Ligand for Electrophillic C-H Activation
William Jones

Justin Rhinehart
Investigations Into the Charge Transfer Mechanism of 4-(Dimethylamino)benzonitrile Using Ultrafast Spectroscopy
David McCamant

Derek Ryan
Self-Assembly and Hydrogelation of Fmoc-Phenylalanine Derivatives
Bradley Nilsson

Ruja Shrestha
Nickel-Catalyzed Conjugate Addition of Organic Halides
Daniel Weix

Student Awards

DEPARTMENT AWARDS

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

John McCreary Memorial Prize
David Kaphan

ACS Rochester Section Award
Jonathan Raybin

ACS Inorganic Chemistry Award
Benjamin Snyder

Merck Index Award
Rebecca Levin

Chemistry Department Award
Matthew DeMars, II
Emily Hart
Katherine Keifer
Emily Redman
Peter Richter

ENDOWED DEPARTMENT FELLOWSHIPS

Robert and Marian Flaherty DeRight Fellowship
Jonathan Chen, Eric Henry Salvatore Priore

Moses Passer Fellowship
Tulaza Vaidya

Elon Huntington Hooker Fellowship
Wesley Asher, Ruja Shrestha

Arnold Weissberger Fellowship
Joshua Brooks, John DiMaio, Jesse Kleingardner, Michael Prinsell, William Spencer

Samuel Allen and Ellen Frances Lattimore Fellowship
Jennifer Ciesielski, Meghan Rodriguez,

Sherman Clarke Fellowship
Nicholas Arnet, Nicole Briglio, Peter Carlsen, John Frost, Zhiji Han, Benjamin Hmiel, Tian Jiang, Yunzhe Jiao, Andrew Kauffmann, Jared Kneebone, Joshua Kolev, Kim Manbeck, Gilbert Reynders, Shaun Shahan, Doug Tusch, Wenwen Yao

COLLEGE AWARDS

Janet Howell Clark Prize
Emily Redman

Presidential Award for Community Service
Emily Hart

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

TEACHING AWARDS

W. D. Walters Teaching Award
Nick Arnett, Jill Caputo, Stephanie Daifuku, Stephanie Dorn

Carl A. Whiteman, Jr. Teaching Award
Faye Gura, Mark Levin, Jonathan Raybin, Emily Redman, Peter Richter

PHI BETA KAPPA

Matthew DeMars, II, David Kaphan, Katherine Keifer, Mark Levin, Rebecca Levin, Maryam Mohammed, Jonathan Raybin, Emily Redman,
Peter Richter

Fellows 11-'12

Ahmed Mohamed Mustafa Abuela
Visiting Graduate Student
Al-Azhar University, Egypt, 2013

Alexey Akimov
Rice University, Texas, 2011

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

William Eckenhoff
Duquesne University, Pennsylvania, 2010

Katarzyna Grubel
Utah State University, Utah, 2011

P.M. Gurubasavaraj
Georg-August University, Germany, 2007

Kiril Igumenshehev
University of Rochester, New York, 2011

Heather Jaeger
University of Georgia, 2010

David Leboeuf
Université Pierre et Marie Curie (UPMC), France, 2005

Andrea Lee
University of Wisconsin - Madison, 2007

Matthew Liptak
University of Wisconsin - Madison, 2008

Run Long
Shandong University, P.R. China, 2008

Kenneth ("Cory") MacLeod
University of British Columbia, Okanagan, 2012

William McNamara
Yale University, Connecticut; Lafayette College, Pennsylvania, 2010

Walter Moss
University of Rochester, New York, 2011

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

Ruth Castro Rodrigo
University of Zaragoza, Spain, 2010

Marie-Pierre Santoni
Universite' de Montre'al, Canada, 2010

Sebastian Schaefer
University of Siegen, Germany, 2008

Alexander Shveyd
Northwestern University, Illinois, 2011

Anni Siitonen
University of Jyvaskyla, Finland, 2010

Hardey Singh
Panjab University, Chandigarh, India, 2008

Brett Swartz
University of Rochester, New York, 2010

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

Kaidong Zhang
University of Manitoba, Canada, 2008

Seminars & Colloquia

JULY 2011

Gerald F. Manbeck (University of Rochester) *"Synthesis and Photoluminescence of Copper(I) Triazole Complexes and Copper(I)/Gold(I) Clusters,"* July 20, 2011

AUGUST 2011

Derek M. Ryan (University of Rochester) *"Self-"Assembly and Hydrogelation of Fmoc-Phenylalanine Derivatives"* August 8, 2011

Michael J. Quinlan (University of Rochester) *"Non-Equilibrium Splits of the Projectile and the Mechanism of Ca + Sn Reactions at 45 AMeV,"* August 18, 2011

SEPTEMBER 2011

Professor Zachary T. Ball (Rice University) "*Catalysis with dirhodium metallopeptides,"* September 9, 2011

Matthew P. McLaughlin (University of Rochester) *"Part I. Apo Azurin and its Mutants as Mononuclear Metal Scaffolds; Part II. Homogeneous Photogeneration of Hydrogen from Aqueous Solutions,"* September 13, 2011

Professor Gary Brudvig (Yale University) *"Learning from Nature: Materials for Solar Fuel Production,"* September 19, 2011

Professor Kristi L. Kiick (University of Delaware) "*Multivalent polymers in the design of hybrid biomaterials,"* September 21, 2011

Hutchison Memorial Lecture

Professor Thomas E. Mallouk (Pennsylvania State University) *"Light Harvesting and Water Splitting in Dye-Sensitized Solar Cells.,"* September 26, 2011

Professor Thomas E. Mallouk (Pennsylvania State University) *"Nanomaterials in One Dimension: Exploring Mesoscopic Phenomena in Template-Grown Nanowires,"* September 27, 2011

Professor Thomas E. Mallouk (Pennsylvania State University) *"Nano-iron Remediation of Contaminants in Soil and Ground Water,"* September 28, 2011

OCTOBER 2011

Professor William B. Tolman (University of Minnesota) *"Using Synthetic Chemistry to Understand Copper Protein Active Sites,"* October 5, 2011

Dr. Lee H. Latimer (Consultant, Pharmaceutical Chemistry) *"Chemistry of ELND006, a Gamma-Secretase Inhibitor for Alzheimer's Disease,"* October 7, 2011

Professor Andrei K. Yudin (University of Toronto) *"Amphoteric Molecules in Organic Synthesis,"* October 14, 2011

Professor Tian Q. Lian (Emory University) *"Wave Function Engineering in Quantum Dots and Nano-heterostructures for Efficient Single and Multiple Exciton Dissociation,"* October 17, 2011

Charles J. Bowerman (University of Rochester) *"Insight into the Principles of Amphipathic Peptide Self-Assembly,"* October 19, 2011

Professor Edward I. Solomon (Stanford University) *"Geometric and Electronic Structure Contributions to Cu/O2 Reactivity,"* October 6, 2010

Professor Emmanuel Lacôte (Institute for Natural Products Chemistry, CNRS, Gif sur Yvette, France) *"The Chemistry of NHC-Boranes,"* October 28, 2011

Professor Gregory Hillhouse (University of Chicago) *"Unusual Reactivity of 2- and 3-Coordinate Nickel: Chemistry Outside the Square Plane"* October 31, 2011

NOVEMBER 2011

Professor Craig Forsyth (The Ohio State University) *"Synthesis and Biology of the Phorboxazole Natural Products,"* November 2, 2011

Professor Bruce Parkinson (University of Wyoming) *"A Combinatorial and Distributed Search for Semiconducting Oxides that Photoelectrolyze Water"* November 3, 2011

Professor David W. McCamant (University of Rochester) *"Mechanisms of Ultrafast Photoinduced Vibrational and Electronic Energy Transfer,"* November 9, 2011

Professor Jerry Yang (University of California, San Diego) *"Recent Applications of Amyloid-Targeting Agents,"* November 11, 2011

Walter Moss (University of Rochester) *"RNA Secondary Structure Discovery and Characterization,"* November 14, 2011

W. Albert Noyes Jr. Memorial Lecture

Professor Martin Head-Gordon (University of California, Berkeley) *"Advances in Practical Density Functional Theory Calculations with Application to Energy Conversion Problems,"* November 15, 2011

Professor Martin Head-Gordon (University of California, Berkeley) *"Strong Electron Correlations in Molecules: Methods and Applications to Tetraradicaloids and Singlet Fission"* November 16, 2011

Professor Martin Head-Gordon (University of California, Berkeley) *"Calculating and Analyzing Intermolecular Interactions,"* November 17, 2011

Professor Mi Hee Lim (University of Michigan) *"Small Molecules as Chemical Tools and Potential Therapeutics for Human Neurodegenerative Diseases,"* November 21, 2011

Nicholas B. Hammond (Rice University) *"1. Investigating the Mechanism of Hoechst 33258 Inhibition of Candida spp. Growth and 2. RNA Internal Loops with Tandem AG Pairs,"* November 29, 2011

DECEMBER 2011

Jennifer L. Rhinehart (University of Rochester) *"Development of Novel Rhodium and Iridium Complexes with a fac-Chelating Ligand for Electrophillic C-H Activation,"* December 5, 2011

Ryan E. Cowley (University of Rochester) *"Three-Coordinate Iron Complexes with Terminal Imido Ligands,"* December 8, 2011

Jing Qiao (University of Rochester) *"Thermodynamic and NMR Structural Studies of RNA Hairpin Loops,"* December 9, 2011

Todd M. Doran (University of Rochester) *"Role of Hydrophobicity, Aromaticity and Turn Nucleation in Peptide Self-Assembly,"* December 12, 2011

Dr. Dmitry Zubarev (University of California, Berkeley) *"Qualitative and Quantitative Quantum Chemistry for Realistic Systems,"* December 12, 2011

Karen P. Chiang (University of Rochester) *"Low-coordinate Iron(I) and Iron(II) Compounds as Model Complexes for Nitrogenase,"* December 14, 2011

Justin M. Rhinehart (University of Rochester) *"Invesigations Into the Charge Transfer Mechanism of 4-(Dimethylamino)benzonitrile Using Ultrafast Spectroscopy,"* December 16, 2011

Dr. Hanning Chen (Northwestern University) *"Time-Dependent Theories for Photo-Induced Processes,"* December 19, 2011

JANUARY 2012

Dr. Jian Liu (Stanford University) *"Understanding Dynamical Properties in Complex Molecular Systems Through a Practical Quantum Approach: From Simple Chemical Reaction Rate to Spectroscopy,"* January 5, 2012

Kaidong Zhang, William Spencer (University of Rochester) *"I. Fingerprint-driven engineering of highly regio- or stereoselective P450 oxidation catalysts; II. Oxidation-Initiated Nazarov Cyclization of Vinyl Alkoxyallenes,"* January 11, 2012

Dr. Ignacio Franco (Fritz Haber Institute - Max Panck Society, Germany) *"Single-Molecule Pulling: Fundamentals and Applications in Molecular Electronics and Molecular Motors,"* January 16, 2012

Dr. Anthony Dutoi (University of Heidelberg, Germany) *"Time-resolved Pump Probe Spectroscopy to Follow Valence Electron Motion,"* January 19, 2012

Dr. Nandini Ananth (California Institute of Technology) *"Novel methods for nonadiabatic dynamics: direct dynamic simulations of electron transfer and proton-coupled electron transfer,"* January 23, 2012

Dr. Paul Zimmerman (University of California, Berkeley) *"Shedding Light on Dark Multiple Exciton States in Acene Crystals,"* January 26, 2012

Arielle Butts (University of Rochester) *"High Throughput Screening for Combination Therapies,"* January 27, 2012

Professor Elon Ison (North Carolina State University) *"Development of Re and Ir Complexes as Catalysts for Oxygen Atom Transfer and C-H Activation/ Functionalization,"* January 30, 2012

Thomas Dugan (University of Rochester) *"A Masked Two-Coordinate Cobalt (I) Complex that Activates C-F Bonds,"* January 31, 2012

FEBRUARY 2012

Seymour Rothchild Lecture

Professor Nadrian C. Seeman (New York University) *"DNA: Not Merely the Secret of Life,"* February 1, 2012

Peter Carlsen (University of Rochester) *"The Development of Pd-Catalyzed Cross-Couplings of Ammonia with Aryl Halides,"* February 3, 2012

Yunzhe Jiao, Lenore Kubie (University of Rochester) *"1. Hydrogen Storage in Metal-Organic Frameworks 2. Bio-nano Interfaces for Solar Energy Applications,"* February 6, 2012

Professor Shannon S. Stahl (University of Winsconsin, Madison) *"Overcoming the Oxidant Problem: Strategies to Use O2 as the Oxidant in Catalytic C-H Oxidation Reactions,"* February 2, 2012

John Frost (University of Rochester) *"Peptide Mediated Asymmetric Catalysis,"* February 10, 2012

Aaron Walsh, Matthew Sharpe (University of Rochester) *"1. Catalytic C-H Functionalization via Iron 2. Removal of Surface Bound Tritium using an Inductively Coupled Plasma,"* February 13, 2012

Wathsala Liyanage (University of Rochester) *"Design and Synthesis of alpha/beta-Peptide Foldamers for Biological Applications,"* February 17, 2012

Mehmet Can (University of Rochester) *"Factors Affecting the Heme Electronic Structure of Proteins with Heme c,"* February 20, 2012

Professor R. Tom Baker (University of Ottawa, Canada) *"Wood Eye! Selective Aerobic Oxidation of C-C Bonds in Lignin Models using Base Metal Complexes: A Comparison of Oxovanadium and Copper Complexes,"* February 20, 2012

Professor Victor Batista (Yale University) *"Studies of Natural and Artificial Photosynthesis,"* February 22, 2012

Yu-Wen Huang (University of Rochester) *"Catalytic Asymmetric Synthesis of Branched Chiral Allylic Esters,"* February 24, 2012

Professor Sophya Garashchuk (University of South Carolina) *"Dynamics of Nuclei in Large Molecular Systems Using the Approximate Quantum Trajectory Framework in Cartesian Space,"* February 27, 2012

MARCH 2012

Steven Jacob (University of Rochester) *"Evolution of a Universal, Bio-Inspired Synthetic Route to Palau'amine and Related Compounds,"* March 2, 2012

Professor Katherine Franz (Duke University) *"Chelation on Cue: Designing Prochelators to Bind Cellular Metal Ions in Response to Disease-Associated Stimuli,"* March 5, 2012

Professor Sam Farid (University of Rochester) *"Revised View of Electron Transfer Dependence on Free Energy,"* March 7, 2012

Professor Eriks Rozners (Binghamton University) *"Synthesis and Properties of Non-Ionic RNA Analogues for Applications in RNA Interference,"* March 9, 2012

Professor Tesuya Satoh (Osaka University, Japan) *"Chelation-Assisted Oxidative C–H Functionalization under Transition-Metal Catalysis,"* March 12, 2012

Yekaterina Lyubarskaya (University of Rochester) *"Nanomedicine: Concepts and Applications,"* March 16, 2012

Professor Troy Van Voorhis (Massachusetts Institute of Technology) *"Exploring Electron Transfer: From Photochemistry to Energy Conversion,"* March 19, 2012

Pu Luo (University of Rochester) *"Mechanism for the Fragmentation of Aryltrialkylstannane Cation Radicals,"* March 20, 2012

Professor Robert Batey (University of Toronto) *"Reaction Development and Discovery: Synthesis of Alkaloids and Heterocyclic Natural Product Targets,"* March 23, 2012

Kelly Sowers (University of Rochester) *"Assembled All-Quantum Dot Films for the Photoelectric Stimulation of Neuronal Action Potential,"* March 26, 2012

Professor Anatoly Kolomeisky (Rice University) *"How Proteins Find and Recognize Targets on DNA: Mechanism of Facilitated Target Search,"* March 28, 2012

Ruja Shrestha (University of Rochester) *"Nickel-Catalyzed Conjugate Addition of Organic Hallides,"* March 29, 2012

APRIL 2012

Andrew S. Kende Distinguished Lecture

Professor Magnus Rueping (RWTH-Aachen University) *"Bio-Inspired Catalysis: From Concepts to Applications,"* April 2, 2012

Professor Magnus Rueping (RWTH-Aachen University) *"Asymmetric Brønsted Acid Catalysis,"* April 3, 2012

Professor Magnus Rueping (RWTH-Aachen University) *"Chiral Counterions in Catalysis,"* April 4, 2012

Hui Wang (University of Rochester) *"Ruthenium Catalyzed Hydroamidation of Terminal Alkynes,"* April 6, 2012

Professor Andrew Moran (University of North Carolina at Chapel Hill) *"Ultrafast Dynamics in Photosynthetic Complexes and Components of DNA,"* April 9, 2012

Sang Min Lee (University of Rochester) *"Organic Light Emitting Devices with Linearly-Graded Mixed Host Architecture,"* April 12, 2012

Professor Armen Zakarian (University of California, Santa Barbara) *"Methods for Asymmetric Alkylation and Haloalkylation of Enolates,"* April 13, 2012

Mary S. Lenczewski (University of Rochester) *"Mechanistic Studies of Benzylsilane and Benzylgermane Cation Radicals,"* April 13, 2012

Randy Sabatini (University of Rochester) *"Development of Dye Sensitized Solar Cells,"* April 17, 2012

William Eckenhoff, Alexander Wotal (University of Rochester) *"1. Solar Energy Conversion to Hydrogen Using Molybdenum Complexes for Proton Reduction 2. No Organometallic Reagents Required: Synthesis of Ketones From Organic Halides,"* April 18, 2012

Wesley B. Asher (University of Rochester) *"Engineering Native and Artificial Heme c Containing Proteins for Biochemical Applications and Studies of Protein Folding,"* April 18, 2012

Professor Valerie Pierre (University of Minnesota) *"Imaging Metal-Induced Oxidative Stress - Inorganic Chemistry to the Rescue,"* April 19, 2012

Professor A. James Link (Prinecton University) *"How to Tie Peptide Knots,"* April 20, 2012

Professor Daniel Gamelin (University of Washington) *"Dopants and Charge Carriers in Colloidal Semiconductor Nanocrystals,"* April 23, 2012

Professor Gabriele Varani (University of Washington) *"Inhibiting RNA with Drug-like Molecules,"* April 25, 2012

Alexander Wotal (University of Rochester) *"Stabilized Anti-aromatic Cations? Making a Case for Hyperaromaticity,"* April 27, 2012

Professor David S. Ginger (University of Washington) *"Nanostructured Photovoltaics: From Conjugated Polymer Morphology to Light Harvesting with Nanoparticles,"* April 30, 2012

MAY 2011

Professor Christopher J. Chang (University of California, Berkeley) *"Molecular Imaging Approaches to Studying Chemistry in the Brain,"* May 2, 2012

Professor Jianmin Gao (Boston College) *"Targeting Membrane Lipids with Designed Peptides,"* May 4, 2012

Sarah Paulson (University of Rochester) *"Hydroaminoalkylation Catalyzed by Group 5 Metal Binaphtolate Complexes,"* May 11, 2012

Barbara Dunlap (University of Rochester) *"New Methods to Measure Anharmonic Coupling using Femtosecond Stimulated Raman Spectroscopy,"* May 14, 2012

Professor Paramjit Arora (New York University) *"A Systematic Approach for Targeting Protein-Protein Interactions,"* May 18, 2012

Nanomaterials Symposium

Christopher Brown (Plextronics Incorporated) *"Plexcore® OC: Aqueous and Non-Aqueous Solution Processed HILs for Organic Electronics Applications,"* May 21, 2012

Professor Duncan Moore (University of Rochester) *"Gradient-Index Optics and Concentrating Photovoltaics,"* May 21, 2012

Professor Richard Hennig (Cornell University) *"Prediction and Design of Materials from Crystal Structures to Nanocrystal Morphology and Assembly,"* May 21, 2012

Professor Kara Bren (University of Rochester) *"Bio-nano Constructs for Solar Fuels,"* May 21, 2012

Professor Greg Scholes (University of Toronto) *"Lessons from Nature about Solar Light Harvesting,"* May 21, 2012

Professor Michael Hickner (Pennsylvania State University) *"New Polymer Membranes for Redox Flow Batteries and Fuel Cells,"* May 21, 2012

Alexander Wotal (University of Rochester) *"Stabilized Anti-aromatic Cations? Making a Case for Hyperaromaticity,"* May 25, 2012

JUNE 2011

Tulaza Vaidya (University of Rochester) *"Electrophilicly-driven Annulations of Polarized Nazarov Precursors with Tricationic Iridium(III) and Heterogeneous Gold Catalysts,"* June 1, 2012

Chemistry-Biology-Biophysics Interface Retreat

Professor Ken Johnson (University of Texas at Austin) *"Role of conformational dynamics in HIV reverse transcriptase nucleotide specificity and the evolution of drug resistance,"* June 7, 2012

Muthiah Manoharan, Ph.D. (Alnylam Pharmaceuticals) *"Making Drugs out of siRNAs,"* June 7, 2012

Jennifer Ciesielski (University of Rochester) *"I. Introduction to Phomactin A, II. The B-Iodoallenolate Cyclization, III. Studies Toward the Synthesis of Phomactin,"* June 25, 2012

Distinguished & Special Lectures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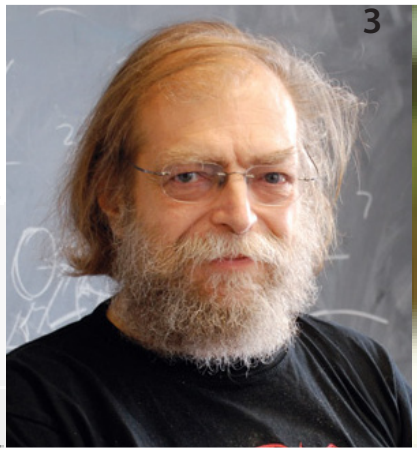
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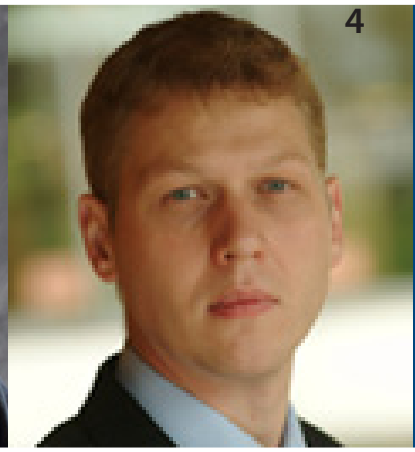
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[1] **Thomas E. Mallouk** Hutchison Memorial Lecture *(September 2011)*
[2] **Martin P. Head-Gordon** W. Albert Noyes Jr. Memorial Lecture *(November 2011)*
[3] **Ned Seeman** Seymour Rothchild Lecture *(February 2012)*
[4] **Magnus Rueping** Andrew S. Kende Distinguished Lecture *(April 2012)*

Staff News

NEWS FROM THE ADMINISTRATIVE STAFF:

The staff enjoyed their annual summer outing by taking a lunch tour on the Canandaigua Lady. The weather was perfect - not raining or too hot! We learned some of the history of Canandaigua Lake and saw some beautiful homes on the water. Thanks to Barbara Snaith for organizing this trip!

BARBARA SNAITH completed her first year with us on July 1st as Administrative Assistant to the Chair of the Department. Through many leaps and bounds, she has satisfied all the demanding challenges placed before her. Some of her many responsibilities include coordinating paperwork as it relates to new faculty recruiting, attending monthly faculty meetings and preparing the discussion minutes. She also manages the immigration obligations needed for the Department's incoming postdoctoral research associates, many of whom are foreign nationals. Barb continues to be a great asset to our Department and enjoys her many responsibilities. In her spare time, Barb enjoys fundraising for causes about which she is passionate, such as the Lollypop Farm, as well as going to the GEVA theatre with her good friends. She is a very active member of her church, chairing fundraisers and women's events. She lives in Gates with her adorable white cat named Snowball!

DEB CONTESTABILE joined the department in February 2012 as our new Undergraduate Studies Program Coordinator and Course Administrator. Previously Deb worked in Pediatrics administration for several years before transitioning to the Medical Center's Family Therapy Training Program, where she worked with graduate and post-doc students for an additional six years. She discovered that she really preferred working on the academic side of the University and decided to focus her career in that direction. Deb also has a strong computer background, including experience with web design, which helped make her a good fit for her new position in Chemistry. Since February, she has been enjoying working closely with Terri Clark and learning the various details of the program, as well as getting to know our faculty and students. She was happy be able to participate in her first Chemistry commencement ceremony and all the preparation it entails. She also completed the CLASP certification training (Continuous Learning for Administrators of Sponsored Programs) so she can assist with grant preparation. She looks forward to a year of learning and growth. Outside of the office, Deb and her husband keep busy with their two boys, ages 10 and 15.

TERRI CLARK started her fifth year this August after having moved into the Development Administrator – Alumni Relations position this past January. She is enjoying working with faculty on grants and awards within the department. Oldest son, Joe, and his wife, Kristy, are expecting their first child in late December. Terri and Ben will be on hand to welcome their second grandchild!

DONNA J. DOLAN is a long time staff member in the Department of Chemistry. She is currently beginning her twenty-fifth year in chemistry, serving as departmental receptionist. In this role, Donna continues to provide support for purchasing in the Chemistry Business Office while also providing assistance to faculty and

managing the chemistry department's main office. In addition, she organizes the departmental distinguished speakers program. Donna is a very proud grandmother, blessed with grandson Austin James, now 20 months old, and on July 7th her daughter Sherry married Andrew Watt, here at the Interfaith Chapel on campus.

Sherry and Andrew Watt

ROBIN COOLEY, our graduate studies coordinator, has now been with the department for eight 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 2012-2013 school year, we are welcoming sixteen new graduate students to the department.

LYNDA MCGARRY (M.S. '85) is the administrative assistant to the chair of the Materials Science program, Todd Krauss, Professor of Chemistry and Optics. Lynda coordinates the graduate student admissions for the interdisciplinary Materials Science program, which welcomes five doctoral and twelve masters degree students again this fall. She also organized the successful "Nanosymposium 2012 –Materials and Processes for Renewable Energy" that was held on May 21, 2012 in Goergen Hall. This past year, the Materials Science program handbook, curriculum and list of faculty from ten departments were all updated to reflect the growing interest in the field. In addition to her Materials Science program duties, Lynda works part-time as an editorial assistant in both the JACS and the JOC offices, and is very grateful to Valerie Fitzhugh and Terrell Samoriski for sharing their enthusiasm and extensive knowledge of the journals. Lynda and her family like to watch lacrosse and spend time at their cottage on Port Bay with family and friends and their schnoodle.

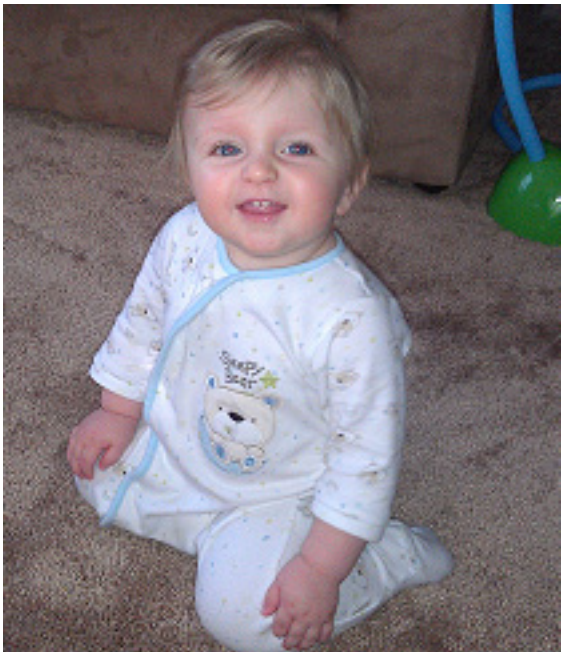
KENNETH SIMOLO (PH.D. '85) starts his twenty-fifth year of service to the University of Rochester. Ken has been assistant chair for administration in the Department of Chemistry since 1988. As assistant chair, Ken manages and advances the administrative and financial functions of the department and also 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 new, ongoing project is the re-writing of the business accounting software for the Department in order to make it web based.

MARGUERITE WESTON, assistant to faculty, has been with the Department of Chemistry for seventeen years. She coordinates Chemistry's 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. Our recent proposal of 2011 was approved by NSF for three-year funding. 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 part-time prepping for the undergraduate general chemistry laboratories. 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 a Master's degree in education. She has clinical experience, having

previously worked in several veterinary clinics prior to coming to the UR. On July 8th, Elly and husband, Brandon, celebrated their son Aaron Timothy's first birthday!

Aaron Timothy York

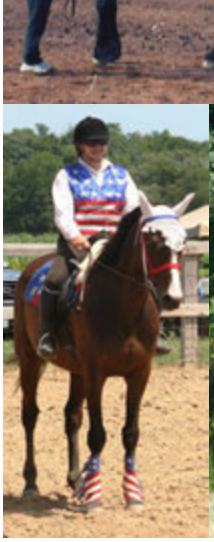


NEWS FROM THE EDITORIAL OFFICES

TERRELL SAMORISKI completed her seventh year as editorial assistant for *The Journal of Organic Chemistry* (JOC) in August 2011. She works closely with Professor Robert K. Boeckman, Jr., associate editor for JOC and continues to enjoy her work in scientific publishing. Her previous position as structure editor for the Chemical Abstract Service also involved the processing of scientific information. She enjoys working with part-time journal assistant **LYNDA MCGARRY (M.S. '85)** whose breadth of scientific knowledge is an incredible resource. The JOC publishes original contributions reporting novel, important findings of fundamental research in all branches of the theory and practice of organic chemistry. In 2011, the Rochester office handled more than 200 manuscripts. As a direct result of the contributions of the JOC Editors and staff, the Thomson Reuters Impact Factor increased to 4.450 and again set a new standard. The journal also has the fastest turn-around rate of manuscripts (from receipt to acceptance) of all the American Chemical Society journals where shorter articles (Notes) and lengthy ones (Articles) are published along with synopses and brief communications. The covers of the journal continue to be a highly desired forum for authors to showcase art relating to their manuscripts.

VALERIE FITZHUGH continues to enjoy working with Prof. William D. Jones as Editorial Assistant with the *Journal of the American Chemical Society* (JACS), and expects that approximately 520 manuscripts will be assigned to this office in 2012. She finds the fast pace of the JACS office engaging and interesting, and the expertise of newer journal assistant, Lynda McGarry, definitely helps expedite the work-flow. JACS, 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. It is the most cited journal in chemistry and received 408,307 total citations and an increase in Impact Factor to 9.907, as reported in the 2011 Journal Citation Reports® by Thomson Reuters. Published weekly, JACS provides research essential to the field of chemistry.

KIRSTIN CAMPBELL, coordinating editor, oversees the staff of *Inorganic Chemistry*. Out of 44 journals in their category, *Inorganic Chemistry*, celebrating fifty years of publishing in 2011, was 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* publishes up to three Forum issues annually, consisting of a set of thematically linked papers from leading scientists on a multidisciplinary topic of growing interest. On a personal note, Kirstin has been busy at home, enjoying and working with her horses. Kirstin has had most of the year off from horse showing due to injury of both horse and rider and has begun training again for dressage, show



Kirsten with William (left) and CK (bottom)

jumping and eventing. Competition this year has been brief but she has enjoyed good results to show for the work thus far. Work will begin next spring breaking two up-and-coming four year old geldings but she looks forward to the challenge. **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.

SCIENTIFIC & TECHNICAL STAFF

TERRY (TED) O'CONNELL starts his thirtieth year with the chemistry department and still enjoys his position as director of technical operations. He is responsible for new equipment installations and any building renovations. This past year, he has been busy training users on the new mass spectrometers that were purchased last year. **JALIL SHOJAIE** is currently a Sr. lab engineer/chemist who works mornings in the chemistry department and afternoons at the University Laboratory for Laser Energetics (LLE). He has been at the University of Rochester since 1996. He worked as a research chemist at the obgyn and anesthesiology departments. His research at the obgyn department involved synthetic and analytical chemistry of trace amount of 3-chlorotyrosine as a bio-marker in premature rupture of membrane in pregnant women. His research at the anesthesiology department was synthetic chemistry of antioxidant drugs for treatment of mitochondrial dysfunctions. Prior to coming to Rochester, he worked as a research chemist at NYU, Nelson Institute of Environmental Medicine (90-95). His research involved synthetic chemistry of cocaine derivatives and development of a crack cocaine aerosol delivery system to study the physiological and behavioral consequences of cocaine and its derivatives. He has peer reviewed research publications and patents both with the University of Rochester and the New York University. His background include applied and basic chemical research, multi-step syntheses of organic, organometallic, analytical chemistry and chemical characterization techniques such as NMR, GC, GC/MS, LC/MS, HPLC, MALDI, FTIR, UV/VIS, and DSC.

ERIC LOBENSTINE (PH.D. '81), manager for computers and network, reports another year of pretty smooth sailing for our computers and network, for which he is glad. He continues to represent Chemistry's interests on numerous IT committees within the University, and finds that he routinely advises IT directors on how various IT initiatives will be viewed at the department level - "in the trenches", so to speak. One major IT push for this year has been Network Registration of computers - designed to help Univ. IT know exactly who is using the computers on our wired networks. He volunteered a small number of department computers for a pilot of the Network Registration process, which helped work out some significant bugs in the system. In July, network registration was implemented on our network for laptops, a process that went (mostly) quite smoothly. In May, Eric finally made the switch to a shiny new email/web server for the department (HP server, mirrored data disks, and Ubuntu Linux) and heaved a sigh of relief that we finally had a modern computer and OS in that role. On the family front, Eric and his wife Jeanne celebrated two UR graduations this year! Brian finished up his MBA at the Simon School, and has headed off to a great job with Parker-Hannifin as a Pricing Trainee. He'll spend a year rotating through different divisions of the company before settling down someplace close, we hope. Ethan finished his double undergrad majors in Music and Brain & Cognitive Science, and has spent part of the summer working with musical theater camps as the Asst. Music Director. He will be studying French and Economics next year as part of the Take 5 program, designed to let students take a fifth year at the UR to broaden their curricular experience, tuition free!

Eric Lobenstine with son Ethan

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 2012, renovations in Hutchison Hall were undertaken: remodeling Dr. Jones lab to include upgrading all of his fume hoods, installed four new 8 foot fume low-flow fume hoods. Cleaned up B25 to make room for the new Mossbauer for Neidigs lab. 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 Johns Hopkins University to watch his daughter play D3 soccer."

In the area of solid-state analysis, crystallographer **BILL BRENNESSEL** continues to offer excellent service. For single crystal analysis (think of sugar or salt crystals, but with more exciting research implications), the X-ray Crystallographic Facility typically examines one new sample per day. This means that the Bruker platform diffractometer with its APEX II CCD area detector is in use continuously. On Fridays, Bill switches hats and runs the CENTC Elemental Analysis Facility, where he determines the amount of carbon, hydrogen, and nitrogen in research samples. Although the instrumentation, a PerkinElmer 2400 Series II analyzer with accompanying AD-6 microbalance, is state of the art, the technique itself is classic. Samples are burned in the presence of oxygen, such that carbon, hydrogen, and nitrogen become carbon dioxide, water, and (after reduction) nitrogen gas. The three gases are then separated and their amounts are measured.

In the spring semester a new group of students in the graduate course in X-ray crystallography (CHM 416) became trained users of the facility. They learned theory and instrumentation, which they will be able to use in their graduate research studies. Students in the undergraduate advanced laboratory techniques course (CHM 234) participated in laboratory experiments in the X-ray facility and also submitted newly synthesized materials to the elemental analysis facility, as part of their education on how to prepare and characterize new molecules. For future synthetic chemists, such experience is invaluable.

Lately Bill has been collaborating with professors from Rochester area colleges, including Professor Bradley Kraft at St. John Fisher College and Professor Michael Coleman at the Rochester Institute of Technology. The cooperative effort that exists is what continues to make Rochester a highly desirable place for chemical education.

SUE CARDINAL, chemistry librarian from the Carlson Library, reports that librarians answer questions through a chat box on our department page: http://www.library.rochester.edu/carlson/home/. Carlson continues adding online access to older journals including *Nature, Science* and the *Journal of Organometallic Chemistry*. We also have unlimited SciFinder access and access to Science Citation Index (Web of Science, ISI) back to 1899. The POA Library has a new director, Tyler Dzuba. He is a recent graduate from the University of North Carolina at Chapel Hill with a BS in Mathematics and Linguistics and a Masters in Library Science. This summer we've added two modular

Computer Studies and Carlson Library

study rooms that we know the workshop(PLTL) groups are going to love, as well as eight new computers, new tables, chairs, carrels and reupholstered comfortable chairs.

NEWS FROM THE BUSINESS OFFICE:

The Business Office continues to provide service to faculty, staff and students on all financial matters such as payroll, reimbursements, purchases, preparation of grant budgets and monitoring grant expenditures. **DORIS WHEELER,** business office manager since 2002, is very happy to report that the business office is running smoothly. The business office staff consists of four members with valuable experience. **ANNA KUITEMS** is responsible for reconciling grant ledgers, P-card management and graduate student payroll, and as backup for Randi Shaw. Anna and her husband, Russell, just purchased a cottage on Silver Lake and have enjoyed spending time there this summer. Their son, Chris, is still in Kazakhstan and their daughter, Megan, left for London this year. Anna and her family plan on visiting her in the fall. **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 27 years now.

DID YOU KNOW...

... that in 2012 the University of Rochester was rated 33rd in the National University category — two notches above its ranking a year ago. Bob Morse, who oversees the U.S. News review, said the UR has edged upward on issues related to its faculty, which include having more teachers with the top degrees in their field and having a low student-teacher ratio in the classroom. U.S. News evaluated about 1,600 colleges and looked at such factors as a college's graduation rate, financial resources and overall reputation in its evaluation.

Instrumentation

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

NMR Spectrometers:

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

Mass Spectrometers:

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

Laser Systems:

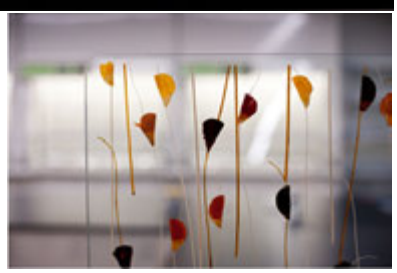
- Transient absorption systems based on a picosecond Nd:YAG laser and a nanosecond excimer-pumped dye laser
- Picosecond time-correlated single photon counting fluorescence system based on a Nd:YLF-pumped cacity-dumped dye laser
- Nd:YAG/dye laser system
- Associated optical instruments:
  monochromators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

Other Instruments Include:

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

Chemistry Librarian Sue Cardinal working with students in the new organic laboratory in Hutchison Hall

A Second Look at the New Organic Chemistry Lab



Last year, the University created an exciting new laboratory in Hutchison Hall for teaching organic chemistry. Incorporated into the new lab is an area for discussion 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 which, in addition to creating a safer work environment, 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.

Departmental Funds

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

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

Chemistry Alumni Research Fund

A general fund that enhances the educational and research activities of the department. The fund enables a number of endeavors, among them the purchase of undergraduate laboratory equipment, assisting graduate students with travel expenses to scientific conferences, and supporting Chemistry's outside speakers program.

Distinguished Lectureship Funds

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

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

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

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

Richard Eisenberg Chemistry Endowment

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

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

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

Magomedov-Shcherbinina Memorial Fund

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

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

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

Marshall D. Gates, Jr. Chair in Chemistry Fund

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

I wish to contribute to the following fund:

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_____ Other - Please specify _____

My gift is in honor of _____ (see above)

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B.S. _____ **PH.D.** _____

ADVISOR

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

Alumni Update

This form is available online at http://www.chem.rochester.edu/alumni/update_contact.php

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

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Department of Chemistry
RC Box 270216
Rochester, New York 14627-0216

585-275-2915 (phone)
585-276-0205 (fax)
alumni@chem.rochester.edu
http://www.chem.rochester.edu/alumni/

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Year degree(s) received from the Department

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NEWSLETTER COMMENTS _____

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