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# Faculty and Staff

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## Greetings to all Department of Chemistry Alumni! We enjoyed a busy and productive 2009-2010 academic year in the Department

and at the University. As I enter my eighth 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.

Inevitably, the economy continues to have an impact upon all of us, and the University of Rochester is no exception. I am pleased to say that it appears that the University will emerge from this period of economic uncertainty stronger than ever. The University continues to make sustaining the quality and distinction of our undergraduate programs its highest priority and has devoted, and continues to devote, a considerable proportion of available resources to help students, and their families, weather these difficult economic times with respect to achieving a college education.

The *very good news* is that this was another record year for applications to the undergraduate program at the College and we enrolled 1174 freshmen in the class of 2014. The Chemistry Department anticipates that a commensurate number of incoming freshmen will participate in the chemistry curriculum. This enrollment growth, coupled with restraints imposed by the economy that have slowed the corresponding growth in the size of the Chemistry faculty, has led to some stresses in terms of the size of Chemistry classes and labs. We hope these stresses will be relieved by the addition of new tenure-track faculty in the coming years. Furthermore, despite an ailing economy, UR Chemistry alumni have remained constant in their generous support of the Department. As has

been the case, the Department remains highly regarded with respect to its sponsored research program.

Like all those involved in basic science research, we are encouraged by the emphasis that our current presidential administration has placed on research and development. The Department of Chemistry's annual sponsored research expenditure exceeded 4.4 million in federal dollars last year. As a top-tier research university and department, we are particularly well positioned to contribute to an expansion of sponsored research, and thus, the education of the next generation of chemistry scholars. We have benefited by the government's efforts to redirect national priorities toward spending more of our nation's gross domestic product on R&D. As a central science, chemistry has an essential part to play in the nation's research enterprise. UR Chemistry faculty have successfully applied for federal funding under the auspices of the American Recovery and Reinvestment Act, as well as other federal and state programs. Last year our Department received funding for three major instruments. Individual faculty received both new and renewed funding for their varied research programs from agencies such as the DOE, NIH, and NSF; junior faculty were successful in competing for funding from the ACS PRF, NSF CAREER, the Alzheimer's Foundation and other Young Investigator awards programs.

As indicated above, the major strategic plan for controlled growth by the University over the next ten years has slowed in pace, although the initial vision remains unchanged. We are confident that UR will continue to make progress in implementing the plan outlined a few years ago, namely an intended growth of approximately 25% in the size of both the undergraduate and graduate student bodies, as well as corresponding growth in the faculty body over the next decade, once the economy stabilizes and improves. We hope that, as part of this growth, Chemistry faculty will increase from 21 to 24-26 over that period. Our goal is to accommodate the already increased enrollments, to expand our faculty expertise in emerging research areas, particularly in areas of emphasis identified during our strategic planning, and to deepen our areas of traditional strength. Fortunately, Chemistry was selected as one of the departments permitted to make a faculty hire this year in perhaps the tightest budgetary year of any of the next few years. We were exceedingly pleased to have attracted one of the top young theorists in the United States, Oleg Prezhdo, from the University of Washington, Seattle. Oleg joined the Department as Professor of Chemistry on July 1, 2010. As Chair, I am pleased to say that proactive efforts

to retain faculty, in an era of increased mobility, have thus far proven successful, although faculty retention, particularly of our cohort of outstanding younger tenured faculty, remains a critical focus going forward.

Chemistry faculty received several notable awards this year, the details of which you will read in this Newsletter. Most notably Rich Eisenberg was elected to the National Academy of Sciences. Rich Eisenberg and I were elected fellows of the ACS, and Bill Jones and I were elected fellows of the American Association for the Advancement of Science. Todd Kraus received the 2009 Goergen Award for Distinguished Achievement and Artistry in Teaching. Rich Eisenberg was honored with the University's Lifetime Achievement Award for his contributions to graduate education over his 34 year career. These kinds of recognition help to sustain our efforts to recruit and retain high quality faculty and students, and enhance the reputation of the Department and the University. Faculty innovation in research, coupled with excellence in teaching, comprise the core of our Ph.D. program, providing a rich environment for the student knowledge and research that is fundamental to science education in the 21st century. Chemistry students, too, received a large number of awards, opportunities, and fellowships last year. Efforts to maintain a cutting-edge in research and education are ongoing, as you will read about in the ensuing pages.

We hope that alumni have taken advantage of Chemistry's newly redesigned website at [www.chem.rochester.edu](http://www.chem.rochester.edu). We hope you found it both useful and informative. We are proud to showcase our department with this informational Internet presence which is now more accessible and utilizes more links, cross references, quick facts, and substantially more graphic detail.

As mentioned briefly above, we were pleased to have been able to make other improvements to our departmental infrastructure this year with the completion of renovations to various labs in Hutchison Hall, including renovation to accommodate the arrival of Oleg Prezhdo and his group. Our two new mass spectrometers (Bruker MALDI-TOF and Thermo-Fisher LC MS), and Bruker EPR spectrometer were purchased, installed and are now fully operational and receiving heavy use.

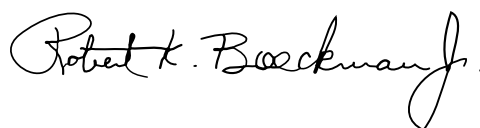
We continue to aspire to grow our graduate program. I am happy to report that this Fall Chemistry will enroll 16 incoming first-year graduate students, about the number sought, after a record number of 31 graduate students entered our doctoral program last Fall. The incoming students bring the total number of graduate students in the Department of Chemistry to 122.

Finally, let me close by thanking all of you for your continuing support of the Department over the years. We are fortunate to have the strong support of the College in all our efforts, however, the support and advice of our alumni is an invaluable resource. We are happy to receive news and proud of your achievements in your respective fields. Please let us know how you are doing by using the reply form at the back of this Newsletter or online at <http://www.chem.rochester.edu/alumni/submitnews.php> and we will pass the word on in next year's edition. Please remember to update your contact information (you may do so now online) as you move from place to place, and stay in touch with your *alma mater*!

One of the defining characteristics of the Department of Chemistry at the University of Rochester is our warm relationship with Chemistry alumni and our collegial atmosphere. Over the years, we have endeavored to establish and nurture the sense of community for our alumni. We encourage you to take this opportunity to acquaint yourself with current members of the Department and reconnect with old classmates, through the Newsletter, through attending events, and through our website. We greatly appreciate your communication and feedback and moreover, want our current students to appreciate the legacy of our extended "Chemistry Family" through a bond with their predecessors. We invite you to visit Rochester, attend Meliora Weekend, and drop by our annual ACS Alumni Social hour typically held in the late afternoon on Monday of the Fall ACS meeting.

Meliora and best wishes to all for a successful and happy year in 2010-2011.

Sincerely,



Bob Boeckman

*The Muses alongside Rush Rhees Library*



# Donors '09-'10

*Includes donations received between July 2009 and June 2010.*

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## CONTRIBUTIONS IN MEMORY OF...

### Magomedov-Shcherbinina Family

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When **HYMAN D. GESSER (POSTDOCTORAL FELLOW '54)** read in the department newsletter last year that Walter Cooper had received the Frederick Douglass Medal he recounted a memorable occasion with Dr. Cooper when they were the winning team in the egg tossing competition during the Chemistry Department picnic, later finding out they had been tossing the raw egg. Hyman and his wife Esther enjoyed over two years in Rochester and in the Noyes lab in the Chemistry Department. Gesser (Ph. D., McGill University) is Professor Emeritus at University of Manitoba.



**WALTER COOPER (PH.D. '57)** was honored by the naming of a Rochester elementary school in his name, the Dr. Walter Cooper Academy. The academy is organized around a set of principles known as Expeditionary Learning. The new school — School 10 — now serves about 100 kindergarten through second-grade students (“Cooper’s Kids”) and will add grades annually through sixth grade. Having a school named for him “imposes upon me a kind of a responsibility to see that the school indeed works,” Cooper was quoted to say. The academy ribbon cutting ceremony was held in November and attended by Bob Boeckman and Debra Haring. Cooper, now retired, enjoyed a long career at Eastman Kodak Company and founded or co-founded

*Walter Cooper at the Ribbon-Cutting Ceremony of RCSD School #10 - Dr. Walter Cooper Academy*



several notable community organizations. He was the first African-American to earn a doctorate in physical chemistry from the University of Rochester. After joining Kodak in 1956, Dr. Cooper rose from research scientist to manager of research innovation and technical communications. In the 1960's, when race riots rocked the city of Rochester, he was a key African-American leader who wrote the original proposal that secured funding for Action for a Better Community, serving as the organization's associate director in 1964. The following year, he served as associate director of the Rochester and Monroe County Anti-poverty Program and was a founding member of the Urban League of Rochester. In recognition of his engagement in civil rights, Dr. Cooper was asked to serve on the New York State Advisory Committee of the U.S. Civil Rights Commission. To enable more opportunities for African-American students, in 1973 he helped found the city's Urban-Suburban transfer program, which still operates today. From 1988 to 1997, he served as a New York State Regent (now Emeritus) and continues to lend his expertise to regent committees today, including the Interstate Migrant Education Council, which advocates for the educational rights of migrant workers' children.

**RICHARD E. PARTCH (PH.D. '63)**, Sr. Professor at Clarkson University, received the 2010 American Chemical Society's E. Ann Nalley Region Award for Volunteer Service. Dick has been a member of ACS for 47 years and has contributed in many significant ways on the local, regional and national levels. He has held many positions of responsibility and is currently an ACS Officer for the Northern New York section, where he has known virtually every high school chemistry teacher in the NNY section.



**ELLIOT RICHMAN (B.S. '70, PH.D. '75)** is the recipient of the 2010 Edward J. Merrill Award, sponsored by the ACS North Jersey Section and the New Jersey Science Teachers Association. The award recognizes outstanding high school chemistry teachers. Richman, who became a teacher as a direct result of the September 11, 2001, terrorist attacks on the World Trade Center and the Pentagon, holds B.S. and





*Elliot Richman receiving the 2010 Edward J. Merrill Award*

Ph.D. degrees in chemistry from the University of Rochester and has been a member of the American Chemical Society since 1975. He has been teaching chemistry and physics in the Ramapo Indian Hills district, Franklin Lakes, NJ, since 2002. "I entered the education profession because I had a deep and thorough knowledge of science—chemistry and physics in particular—and a desire to share it in a meaningful way, so I turned to the education of young people," Richman said, "and I have not regretted this decision." What goes into outstanding teaching of chemistry? More than you might think. For example, Richman incorporates reading and writing in his science classes. "Because words are the tools with which most people think," says Richman, "we need to learn to use them well in all areas." He is also a proponent of reading, especially biography. "Students who may not relate to scientific concepts and mathematical relationships nonetheless enjoy learning about the movers and shakers who made the great discoveries," he explains, "and this human aspect of science often motivates students to learn the course content and enhances their overall enjoyment of science." Richman has found that giving students this perspective makes the science more accessible to them and encourages them to overcome difficulties they encounter in understanding or mastering the scientific ideas themselves.

In recognition of a career spanning three decades that includes pioneering contributions to organic chemistry, chemistry professor **DENNIS P. CURRAN (PH.D. '80)**, received an honorary doctorate from France's eminent University of Pierre and Marie Curie during a March 26, 2010 ceremony at the Sorbonne in Paris. Curran, a Distinguished Service Professor of Chemistry at the University of Pittsburgh, was one of eight scientists worldwide to receive honorary doctorates from the University of Pierre and Marie Curie in Paris, the leading scientific and medical research institu-

tion in France. Curran has written approximately 400 papers, has been granted 30 patents, and has published two books since 1981. He is the founder of Fluorous Technologies, and is noted for developing a process by which complex molecules can be developed from simple organic materials, allowing for faster generation of new chemical

compounds. The process, known as fluorous synthesis, has led to several anticancer agents, including one undergoing clinical trials. While a doctoral student at the University of Rochester, Dennis worked under the direction of Andy Kende.

*Dennis P. Curran*



**CLIFF KUBIAK (PH.D. '80)** was part of the Navy's Distinguished Visitor Program in July of 2009. He was invited



to take a C-2A Greyhound transport plane out of the San Diego Naval Base to join the USS Nimitz nuclear aircraft carrier, already underway. This incredible opportunity came through a chance encounter with the Public Affairs Officer for the Nimitz in the Providence, RI airport. His

certificate designated him as a NAFOD – No Apparent Fear of Death.

**THOMAS R. SIMPSON (PH.D. '94)**, Associate Director of Medicinal Chemistry with AstraZeneca (Wilmington, DE), revealed the structure of AZD2624, a drug candidate that reached Phase II clinical trials in patients with schizophrenia. Schizophrenia affects about 1% of Americans over the age of 18, according to the National Institute of Mental Health. Patients with the disease typically take drugs with a mixture of activities, including blocking dopamine D2 receptors in the brain. But the drugs have side effects and don't treat all of schizophrenia's symptoms.

Adjusting dopamine levels in the brain by an indirect mechanism could address some of those issues, Simpson explained. He and his coworkers learned that blocking the neurokinin-3 receptor (NK3r), a G-protein-coupled recep-

*continued on next page*

tor in the brain, might help, so they decided to pursue this strategy. Simpson and colleagues took inspiration from talnetant, a quinoline NK3r blocker developed by Glaxo-SmithKline that reached Phase II clinical trials for schizophrenia before being discontinued. They sought to improve talnetant's solubility, among other properties. One of the team's more promising quinolines had a sulfonate ester substituent that was susceptible to hydrolysis. Replacing the sulfonate ester with an alkylsulfonylamino group not only eliminated the hydrolysis problem but also led to improvements in solubility. This fine-tuning led the AstraZeneca team to AZD2624. In animal tests, AZD2624 led to an increase in dopamine levels in the brain, an effect that's thought to be helpful for treating schizophrenia. In Phase I clinical trials in healthy people, high doses of AZD2624 had a significant side effect—reductions in testosterone levels. So a Phase II clinical trial was set up to evaluate the efficacy of a dose that didn't have that side effect. Unfortunately, that dose did not lead to robust improvements in schizophrenia symptoms in the Phase II trial, so AstraZeneca discontinued development of AZD2624 in 2009. However, they are continuing to explore AZD2624's possible use as a neuroendocrine modulator and other avenues in which it might benefit patients.

Born in Kabul, **AWISTA AYUB (B.S. '01)** escaped with her family to Connecticut in 1981, when she was two years old. An athlete her whole life, she was inspired to start the Afghan Youth Sports Exchange after September 11, 2001, as a way of uniting girls of Afghanistan and giving them hope for their future. She chose soccer because little more than a ball and a field is needed to play; however, the courage it would take for girls in Afghanistan to do this would have to be tremendous - and the social change it could bring about by making a loud and clear statement for Afghan women was enough to convince Awista that it was possible.

Under Taliban rule, girls in Afghanistan could not play outside of their homes, let alone participate in a sport on a team. In 2003, Awista founded the Afghan Youth Sports Exchange, a non-profit organization dedicated to preparing Afghanistan's youth with leadership skills required to promote athletics in their schools and communities. With AYSE sponsorship, Awista brought eight girls from Afghanistan to the United States for a soccer clinic, in the hope of not only teaching them the sport, but also instilling confidence and a belief in their self-worth. They returned to Afghanistan and spread their interest in playing soccer, making it the first international girls soccer team from Afghanistan. In 2006, Ayub brought Afghan-American coaches to Afghanistan to organize a girls soccer clinic, working with more than 250 girls through the auspices of the Af-



*Awista Ayub at the University of Rochester*

ghanistan National Olympic Committee. Two Afghan female soccer players sponsored by AYSE received the Arthur Ashe Courage Award at the 2006 ESPYs. What began with eight young women has now exploded into something of a phenomenon. Fifteen teams now compete in the Afghanistan Football Federation, with hundreds of girls participating. Against all odds and fear, these girls decided to come together and play a sport that has reintroduced the very traits that decades of war had cruelly stripped away from them - confidence and self-worth.

Ayub is a 2001 graduate of the University of Rochester and 2002 Take-5 Scholar. She also has an M.P.A. from the University of Delaware. From 2005 to 2007, she served as the Education and Health Officer at the Embassy of Afghanistan in Washington. In *However Tall the Mountain*, published in September, 2009, Awista tells both her own story and the deeply moving stories of the eight original girls, describing their daily lives back in Afghanistan, and how they found strength in each other, in teamwork, and in themselves - taking impossible risks to obtain freedoms we take for granted. This is a story about hope, about what home is, and in the end, about determination. As the Afghan proverb says, "However tall the mountain, there's always a road."

**JASON G. GILLMORE (PH.D. '03)** received an NSF Career Award and was promoted to Associate Professor at Hope College in Holland, MI. After completing his B.S. and M.S. degrees at Virginia Polytechnic Institute, he decided to pursue his doctorate in physical organic chemistry at UR with Prof. Joe Dinnocenzo. He worked in collaboration with Prof. Tom Brown in the Optics department as well as renowned photochemist Dr. Samir Farid and polymer chemist Dr. Doug Robello at Kodak. An opportunity to mentor an undergraduate researcher during this time

convinced Gillmore of his desire for a faculty career at a research-intensive undergraduate institution. After completing his Ph.D. in 2003, Dr. Gillmore pursued a short NIH postdoctoral traineeship in the labs of Prof. Ned Porter at Vanderbilt University then joined Hope College in 2004.

**MARTIN T. ZANNI (B.S. '94)**, Meloche-Bascom Associate Professor of Chemistry, University of Wisconsin, Madison, along with Sang-Hee Shim, received the ACS Nobel Laureate Signature Award for Graduate Education in Chemistry, 2010. Their research has revolutionized the technology of two-dimensional infrared spectroscopy, performing groundbreaking studies of amyloid fibers. Zanni is the recipient of numerous awards, including the 2001 ACS Nobel Laureate Signature Award for Graduate Education in Chemistry for his Ph.D. work



as a student under the guidance of Daniel M. Neumark at UC Berkeley. Zanni is the first to receive this award as both student and mentor.

**JAVIER VELA (PH.D. '05)** joined the faculty of Iowa State University in August 2009 as an Assistant Professor. He received his Ph.D. from the University of Rochester in 2005 working with Prof. Patrick L. Holland, and was a Postdoctoral Researcher at the University of Chicago from 2005 – 2006 with Prof. Richard F. Jordan. From 2007 – 2009 he was Director's postdoctoral fellow in the team of Jennifer A. Hollingsworth and Victor I. Klimov at Los Alamos National Laboratory.

**LEA VACCA MICHEL (PH.D. '06)** just completed her first year as Assistant Professor of Chemistry at Rochester Institute of Technology. Lea joins other UR alumni, **CHRISTOPHER COLLISON (POSTDOCTORAL FELLOW '00)**, now an assistant professor of physical chemistry and **CHRISTINA COLLISON (PH.D. '01)** and **JEREMY CODY (PH.D. '99)**, now both assistant professors of organic chemistry. Also on faculty at RIT is **LAURA TUBBS (PH.D. '82)**, a professor of nuclear chemistry.



**BRIAN R. MCNAUGHTON (PH.D. '07)** has accepted a faculty position in the Chemistry Department of Colorado



State University. Three long-standing and critical challenges in the field of chemical biology are: (1) The development and application of high-throughput methods that identify small molecule - RNA interactions, which result in the regulation of an RNA's cellular function; (2) The design and synthesis of molecules that selectively bind a targeted protein surface, and disrupt a targeted protein-protein interaction; and, (3) The development and application of high-throughput methods to identify molecules and reagents capable of targeting the delivery of small molecule, macromolecule, and nanoparticle therapeutics and bio-imaging reagents to diseased cells and tissue. Researchers in The McNaughton Group address these challenges using methods in organic synthesis, combinatorial chemistry, molecular biology, and cell biology, in the context of high-throughput screening and evolution-based selections.

In June 2010 **KUMIKO TANAKA (B.S. '07)** embarked on a new 5-week adventure to India, participating in a volunteer program with Sahara For All (SFA). SFA is a social based non-government, non-profit and non-political organization, established in 2003 for the development of deprived and destitute people in the remote area of Orissa, one of the most underdeveloped states of India. Since graduation from UR, Kumiko has been working at the Broad Institute in Cambridge, MA, putting her chemistry degree to good use while working in the cancer genomics lab of Matthew Meyerson. There, Kumiko presented her work at the Institute's internal conference and poster session and also published twice (in *Nature* and *Cancer Biology & Therapy*) with the Meyerson group. As a B.S. Chemistry major, Kumiko conducted her senior thesis research in the laboratory of Professor Bradley Nilsson. She also worked in the Department's development office as a student assistant. Kumiko started medical school at USC this fall.



**JOHN BERTOLA (B.A. '09, M.S. '10W)** had an eventful year as a Noyce Scholar in the Warner School of Education at the University of Rochester. After graduating in 2009, John decided to pursue his Masters degree in science education. The Robert Noyce Teacher Scholarship Pro-



gram is an NSF-funded program that encourages talented science, technology, engineering, and mathematics majors to become K-12 STEM teachers. The program provides funding to institutions of higher education to support scholarships for undergraduate STEM majors and post-baccalaureates, enabling them to earn their teaching credentials, on the condition that they commit to teaching in high-need K-12 school districts within six years of receipt of the Masters degree. The 15-month course of study was a concentrated program, involving pedagogical coursework in addition to practicum studies, student teaching, and community outreach. John, Chemistry student assistant extraordinaire, designed and implemented the Chemistry website, and other key web-based technology, in addition to working on numerous publications, projects, and events for the Chemistry Department during his 5-year long service as a student employee. The systems that John developed for Chemistry were so well received that he was recently hired by the UR Deans' Office as a Senior Analyst for the School of Arts, Sciences and Engineering. John will work at UR for a year or two on some innovative web-based projects before embarking upon his teaching career.

## IN MEMORIAM

As this newsletter went to press, we were saddened by the news that **PROF. JACOB BIGELEISEN**, former Chair of the Chemistry Department here at UR from 1970-1975, passed away at the age of 91. He is survived by his wife, Grace Bigeleisen of Arlington, VA and his son, Paul Bigeleisen, Prof. of Anesthesiology at UPMC Presbyterian in Pittsburgh, PA.

**PAUL E. FANTA (PH.D. '46)**, an emeritus professor of chemistry at Illinois Institute of Technology (IIT), passed away May 10, 2010 at the age of 88. Born in Chicago, Fanta earned a bachelor's degree in chemistry from the University of Illinois, Urbana-Champaign, in 1942 and a doctorate in chemistry from the University of Rochester in 1946. After spending a year as an instructor at Harvard University, Fanta joined the chemistry faculty of IIT in 1948 where he stayed until retirement in 1984.

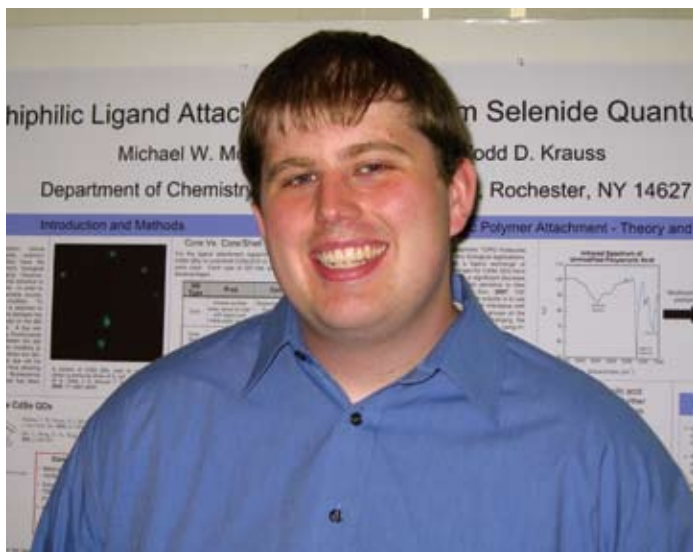
Professor Fanta's skill in the classroom and the laboratory earned him academic acclaim and broadened not just his horizons but those of his family. The gifted researcher and professor earned visiting fellowships in London, Prague, Moscow and Nottingham, England. And while he was enriched by the academic rigors, his family reaped the benefits of many multicultural experiences. "We lived in cities and cultures so different from our own," said his wife of 60 years, LaVergne. "We had adventures enough to fill a lifetime."

The Chemistry department lost a dear friend last year. **SYLVIA ROSNER ROTHCHILD**, the widow of **SEYMOUR ROTHCHILD (PH.D. '48)** passed away in the spring of 2009 at the age of 86. Through the generosity of Sylvia and the Rothchild Family Foundation, a Distinguished Lectureship was established in memory of Seymour (1920-2001). Sylvia was an accomplished woman in her own right. The daughter of European immigrants, she was raised and edu-



cated in Brooklyn, NY. Although a scientist by early training, she went on to become a much sought-after lecturer, in addition to an author, editor, amateur painter, and cellist. A prolific writer throughout her lifetime, she published a novel, a biography, personal essays, book reviews and articles, and two well-received oral histories: one

a compilation of interviews with Holocaust survivors and the other featuring the experiences of Soviet Jewish émigrés. At the same time, she was a consummate and gracious homemaker, wife and mother. Sylvia and Seymour married in 1944 and moved to the Boston area after World War II, where their three children were born. Seymour, who while at the University of Rochester earned his doctoral degree in chemistry under the direction of Virgil Boeckelheide, went on to found New England Nuclear Medicine. Both Sylvia and Seymour shared a passion for music: he played the violin and she the cello. Over the years, they performed with the Sharon Civic Orchestra, the Boston Civic Orchestra, and the Boston Philharmonic Orchestra. The Rothchilds were extremely engaged in their community and supported numerous Jewish organizations, as well the arts and music, in addition to their generous endowment to the Department of Chemistry. Sylvia and Seymour are greatly missed by those who knew them - it is envisioned that, with the Lectureship that bears the Rothchild name, their memory will live on for future generations in Rochester.



*Michael W. McCoy*

**MICHAEL W. MCCOY (B.S. '08)**, of Madison, Wisconsin, passed away April 24, 2010, at the age of 25. Michael was born March 15, 1985, and raised in Amherst, MA, the son of Susan and William McCoy. He attended Amherst public schools and graduated from Amherst Regional High School's Class of 2003. He graduated from the University of Rochester in 2008 with a B.S. in Chemistry. After a fifth year in the UR "Take Five" program to pursue an interest in linguistics, Michael had begun working toward his Ph.D. in Materials Chemistry at the University of Wisconsin, having just completed his second year.

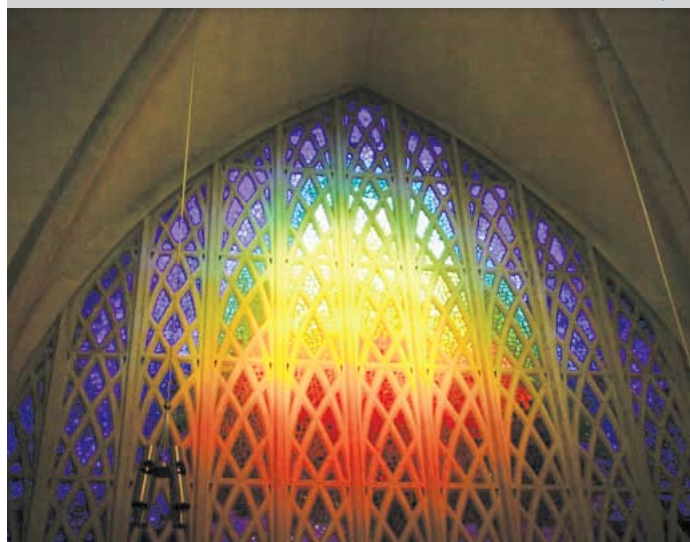
Mike loved learning, reading literature, writing essays and poetry, critiquing movies, and watching silly TV comedies. He loved planning theme parties, making CD music mixes, and watching sports. Most of all, he had a huge heart and loved hanging out with his friends and family. Mike is survived by his parents and a younger brother, Christopher, who just received his B.A. in 2010 from the University of Rochester. A memorial fund has been established at the University of Wisconsin to recognize graduate students in materials chemistry who best exemplify Mike's love of life, people, and chemistry. The Department of Chemistry, with his friends and family, mourns his untimely death. Michael, we will miss you.

**ALTHEA LAWSON**, a valued member of our housekeeping staff, died February 8, 2010, at the age of 52. Althea is remembered by friends, relatives, and all of us, as a warm, giving person who always had a kind word. She had recently celebrated ten years of service with the University of Rochester (2009) and we here in the Chemistry Department were grateful recipients of her hard work and dedication. Althea, you are greatly missed!

*The Department of Chemistry also mourns the passing of:*

- ☞ Elinor Brooks (B.A. '39)
- ☞ Margaret L. Rathbun-Ames (B.A. '39, M.D. '43)
- ☞ Walter Keleher (B.A. '40)
- ☞ Stephen Mayka (B.A. '40)
- ☞ J. Donald Urquhart (B.S. '40)
- ☞ June Buckley (B.S. '41)
- ☞ Richard Conyne (B.A. '41)
- ☞ Jane Marvin ('41)
- ☞ Jean P. Terry (B.A. '41)
- ☞ Irving B. Joffe (B.S. '42)
- ☞ Jane D. Lough (M.S. '49)
- ☞ Guido V. Marinetti (B.S. '50, Ph.D. '53)
- ☞ Claire Johnston (B.S. '50)
- ☞ Peter J. Hawkins (Postdoc. '52)
- ☞ Bruce J. Dropesky (Ph.D. '53)
- ☞ Charles T. Genaux (M.S. '53)
- ☞ Lester L. Lansky (B.A. '54)
- ☞ Louis G. Daignault (Ph.D. '57)
- ☞ Jerrold A. Koeplin (B.S. '57, M.S. '62)
- ☞ Charles P. Kuimjian ('57)
- ☞ Seth H. Lourie (B.A. '59)
- ☞ Doris Berry (B.S. '60)
- ☞ Roger W. Crecely (B.S. '64)

*Interfaith Chapel*



## Richard Eisenberg receives Multiple Honors



*Bruce E. Bursten, ACS Past President, and Richard Eisenberg at his formal election as a Fellow of the American Chemical Society*

2009-2010 was a great year for Rich Eisenberg. Rich, the Tracy H. Harris Professor of Chemistry was elected to the National Academy of Sciences, one of the highest honors that can be accorded to a scientist, and received the University of Rochester Lifetime Achievement Award for Graduate Teaching. He was also elected to the American Chemical Society as a Fellow and was inducted into the American Academy of Arts and Sciences.

The National Academy of Sciences is an honorific society of distinguished scholars engaged in scientific and engineering research, dedicated to the furtherance of science and technology and to their use for the general welfare. Members are elected annually in recognition of their distinguished achievements in original research. Of the approximately 2,100 members and 380 foreign associates, nearly 200 have won Nobel Prizes.

The Lifetime Achievement Award in Graduate Teaching commemorates the distinguished careers of University of Rochester faculty members who have, throughout a significant portion of their career, provided outstanding guidance

and mentorship to doctoral students at the University, and whose students have in turn gone on to make important contributions in scholarship, business, or government that flow from their doctoral studies. This prestigious award was presented at the Doctoral Commencement Ceremony in May of 2010.

Rich has been honored for his contributions to the fields of inorganic and organometallic chemistry, and as a researcher, teacher, leader, and mentor. He has given talks all over the world, most often as an invited distinguished lecturer. He has been the recipient of numerous prestigious awards throughout his career attesting to the esteem in which he is held by his colleagues on local and national levels.

In addition to being a stellar scientist, a creative and penetrating intellect, and a dedicated teacher and mentor, Rich is an exceptionally active and good citizen of the chemistry community, exemplified by his long and distinguished service to the American Chemical Society. His contributions alone as Editor-In-Chief of *Inorganic Chemistry*, the

leading journal in its field, have been an enormous force on the direction of the field since 2001. He has also served as Chair of the Inorganic Division, Chair of the Organometallic Subdivision, Chair of the Gordon Research Conference on Organometallic Chemistry, and as a member of the Editorial Advisory Boards of the *Journal of the American Chemical Society*, *Inorganic Chemistry* and *Organometallics*. He currently serves on the Editorial Advisory Boards of *Accounts of Chemical Research* and the Scientific Advisory Board of the NSF Center for Chemical Innovation (CCI) on "Powering the Planet." He received the ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry in 2003, and was elected a Fellow of the American Association for the Advancement of Science in 2005.

Rich received his undergraduate and graduate degrees from Columbia University. In 1973, he joined the faculty of the University of Rochester. His research interests are in inorganic and organometallic chemistry, photochemistry relating to solar energy conversion, and catalysis. Some of his specific research activities include the study of new luminescent square planar complexes and their incorporation into molecular assemblies for photoinduced charge separation and artificial photosynthesis, the development of parahydrogen induced polarization for hydrogen addition reactions, the discovery of new luminescent gold and platinum group element complexes for application in electroluminescent

*Richard Eisenberg in the laboratory*



devices, and the design of new electrophilic catalysts for electrocyclizations and tandem organic transformations.

Eisenberg's research has placed him in the spotlight of inorganic chemistry throughout his career. During the past five years, his work has become even more visible as it applies to fundamental chemistry vis-a-vis the ever growing energy needs of our nation and the world. His interests are broad and his contributions to small molecule activation, coupled with his extensive training in photochemistry, have paved the way to what now seems to be his most impressive area: light to energy conversions in synthetic systems as robust analogues of photosynthesis. A distinctive attribute of Eisenberg's chemistry research is the integration of synthesis, spectroscopy, structural characterization, reaction chemistry, kinetics and mechanistic analysis for new compounds and reaction systems in the advancement of science and technology, most recently in the area of converting solar energy into non-carbon fuels.

In the midst of these far-reaching contributions, Rich Eisenberg's teaching, research, and intensive mentoring activities have never faltered. Eisenberg has served as doctoral thesis advisor for more than 36 graduate students, as a postdoctoral mentor for a similar number of postdoctoral fellows, as well as senior and summer research advisor for more than 25 undergraduate students. He is first and foremost an academician. He has served as an untiring advocate for inorganic chemistry and the critical interplay between teaching and research. He has been an unwavering proponent of the importance of the integration of research and teaching at all educational levels from undergraduate to postdoctoral fellows. Rich taught general chemistry with distinction for 25 years. He strongly influenced the shaping of the undergraduate and graduate curriculum in the subdiscipline of inorganic chemistry at Rochester. Prior to his arrival, inorganic chemistry had not been recognized as a distinct subdiscipline. It can rightfully be said that he is the father of inorganic chemistry at Rochester.

Rich commands great affection, respect, and admiration from his former students, postdoctoral fellows, and colleagues alike.

**CONGRATULATIONS RICH!**

# Robert K. Boeckman, Jr. and William D. Jones elected as Fellows of the American Association for the Advancement of Science

**Robert K. Boeckman, Jr.** (Chair and Marshall D. Gates, Jr. Professor of Chemistry) and **William D. Jones** (C.F. Houghton Professor of Chemistry) were elected as Fellows to the American Association for the Advancement of Science (AAAS) in recognition of their meritorious efforts in the advancement of science and its applications. The AAAS is an international non-profit organization dedicated to advancing science around the world by serving as an educator, leader, spokesperson and professional association. In addition to organizing membership activities, 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.

## Robert K. Boeckman, Jr.

“Bob has been at the forefront of discovering improved methods for the synthesis of organic compounds for many years,” says Joanna Olmsted, dean of the College Faculty of the University. “It is wonderful and fitting that the American Association of Advancement of Sciences has recognized his contributions this way.”

Boeckman was also elected to the Fellows Class of 2009 of the American Chemical Society. This is an honor bestowed upon scientists who have made outstanding contributions to both chemistry and to ACS.

Boeckman’s research has focused on new ways to construct complex organic molecules controlling the three-dimensional spatial arrangement of atoms. He develops and employs new organometallic chemistry to selectively construct or transform complex molecules. Using the methods developed by Boeckman, organic chemists are able to construct complex molecules possessing precise three-dimensional structures that can function as molecular probes of the interaction of small molecules with proteins and nucleic acids. The molecules can serve as prototypes or leads in the development of human pharmaceutical agents.

Boeckman earned his doctorate in chemistry from Brandeis University and was a professor of chemistry at Wayne State University in Detroit before coming to the University of Rochester in 1980. In 2002, he was named the Marshall D. Gates Jr. Professor of Chemistry and has chaired the Department of

Chemistry since 2003. He has been chair of the Organic Division of the American Chemical Society, and is currently an associate editor of the *Journal of Organic Chemistry*, and the vice president of Organic Syntheses, Inc., a nonprofit organization that publishes selected organic synthetic procedures that are independently checked for use by the organic synthesis research community in academia and industry. As part of the inaugural class of Fellows, he was recently named a Fellow of the American Chemical Society. Among his awards are the ACS Arthur C. Cope Scholar Award, an A. P. Sloan Fellowship, and a National Institutes of Health Career Development Award.

A member of the Rochester faculty since 1980, Prof. Boeckman has devoted his research career to developing new tools that pharmaceutical companies can use in the discovery and development of new drugs. His work on the three-dimensional design of complex organic molecules is widely recognized for giving researchers new avenues for designing drugs that can create a desired effect while minimizing harmful side effects. The Boeckman research group has been active in the development of new synthetic strategies and methods, and the application of this chemistry to the stereocontrolled synthesis of complex molecules of natural origin. These efforts have spanned a structurally diverse group of natural products including terpenes, alkaloids, polyether ionophores, macrolides, anthracyclines, as well as complex tetramic and tetronic acids. The Boeck-

*Robert K. Boeckman, Jr.*





man group's efforts incorporate tests of physical principles and theory in order to provide deeper insights into the design and implementation of stereocontrolled synthetic reactions. He has been a leader in this mainstream field of organic chemistry, and his work enjoys worldwide impact. He has coauthored more than 120 research papers, reviews, and book chapters, principally in the area of synthetic organic chemistry.

## William D. Jones

Prof. Jones was also elected as a Fellow to the American Chemical Society. This is an honor bestowed upon scientists who have made outstanding contributions to both chemistry and to ACS.

Prof. Jones is one of the leading organometallic chemists of his generation. His discovery of rhodium complexes that react with carbon-hydrogen (C-H) bonds in simple unactivated alkanes in homogeneous solution at ambient temperatures is a major landmark in organic chemistry. In addition, his isotope labeling and isotope effect experiments mapped out the potential energy surface for the energetics of C-H bond activation, resulting in an understanding of both the kinetic and thermodynamic bases for activation of a wide variety of hydrocarbons. He has also published some of the first kinetic evidence for the formation of transient complexes formed between alkanes and metals during the activation of aliphatic C-H bonds.

Prof. Jones has made important contributions to the activation and functionalization of carbon-carbon (C-C) bonds. He has discovered examples of metal-catalyzed reactions of C-C bonds that include metathesis, hydrogenolysis, and carbonylation. Further, he has discovered metal complexes that can cleave aryl-cyanide and aryl-acetylide bonds, the former being a critical step in the DuPont process for making nylon. These studies have made Prof. Jones one of the most respected investigators in the interdisciplinary area of organic and inorganic chemistry. Jones is a major contributor to our understanding of how metals can be used to cleave the most stable bonds in organic molecules.

Prof. Jones has also worked on several other key problems involving metal-mediated cleavage of strong bonds, including carbon-sulfur (C-S) and carbon-fluorine (C-F) bonds. For example, C-S bond cleavage is a key reaction in desulfurization of fuels. Jones has developed a nickel hydride dimer that desulfurizes dibenzothiophene, one of the most intractable sulfur-containing impurities, to a nickel biphenyl derivative that undergoes hydrogenolysis to biphenyl with regeneration



*William D. Jones*

of the active Ni dimer. This work has the potential to lead to new, efficient desulfurization catalysts that may provide an important advance in environmental chemistry.

As for C-F bond activation of fluoroalkanes, Prof. Jones has discovered that  $\text{Cp}^*_2\text{ZrH}_2$  is capable of cleaving a wide variety of aliphatic C-F bonds, generating  $\text{Cp}^*_2\text{ZrHF}$  and the reduced hydrocarbon. No other transition metal-based system has shown this type of reactivity.

Recently, Prof. Jones has taken a leadership role in the new NSF Center for Enabling New Technologies through Catalysis (CENTC), which was awarded \$15 million over the next five years and supports collaborative research among 15 principle investigators at ten institutions. Prof. Jones is currently working on a collaborative project that explores non-platinum metal systems (Rh and Ir) for Shilov-type hydrocarbon activation and functionalization. Another collaborative project examines metal systems where electrochemical oxidation of a compound known to activate methane might permit nucleophilic attack/functionalization. This latter project has potential applications in a methane/methanol fuel cell.

Jones earned his doctorate in chemistry from the California Institute of Technology in 1979 before coming to the University of Rochester in 1980. Since then he's been the recipient of the John Simon Guggenheim Fellowship, Fulbright-Hays Scholarship, a Royal Society Guest Research Fellowship, and two awards from the American Chemical Society.

# Todd Krauss receives the 2009 Goergen Award for Distinguished Achievement and Artistry in Undergraduate Teaching

Professor Todd Krauss was awarded the 2009 Goergen Award for Distinguished Achievement and Artistry in Undergraduate Teaching. The Goergen Award recognizes the distinctive accomplishments and skills of individual teachers in undergraduate courses in the College. The Award aims to acknowledge the full scope of work that contributes to excellence in undergraduate education. It can be given for distinguished teaching in large introductory courses or advanced seminars. In addition to being given for superior classroom performance, it can recognize innovation in course design or teaching methods, the creative use of educational technology, the integration of research and teaching, the capacity to elicit superior work from students, or other pedagogical skills.

Todd became a full Professor this past year at the University of Rochester. He received both his Bachelor's degree in Applied and Engineering Physics and his M.S. and Ph.D. degrees in Applied Physics from Cornell University (1991/1994/1998), the

*Todd Krauss with wife, Lisa*



latter two under the direction of Professor Frank W. Wise. He completed his postdoctoral training at Columbia University under the direction of Prof. Louis E. Brus before joining our faculty at Rochester in the summer of 2000; in 2006 he was also named Professor of Optics.

Since commencing his appointment at Rochester in 2000, Todd rapidly developed an impressive research program in nanometer scale materials and devices. His multidisciplinary approach spans many new and exciting areas such as fundamental studies of the optical and electronic properties of carbon nanotubes and semiconductor quantum dots, biomedical and renewable energy applications based on carbon nanotubes and semiconductor quantum dots, and the underlying forces responsible for protein folding. He is a rising star in the field of nanomaterials, ranked at the top of his peers for his work on carbon nanotube photophysics. His forward-looking research program, on par with that of the leading individuals in the field, has made a significant impact in two distinct sub-areas of nanomaterials physical chemistry: the photophysical properties of both carbon nanotubes and colloidal semiconductor nanocrystals (NCs). Most recently, he discovered a new class of NCs that do not exhibit fluorescence blinking, solving a 15-year old puzzle. In addition, Krauss leads a growing effort in biophysical and bioanalytical chemistry, and based on this work has established a startup with five employees working with Strong Hospital on detecting pathogens in urine. Krauss chairs the NanoOptical Materials Cluster. In May of 2009, he organized, on behalf of Deans Robert Clark and Stephen Dewhurst, a highly successful and well attended two-day symposium highlighting UR initiatives in nanomaterial applications in renewable energy and biomedicine.

Prof. Krauss' research group has attracted a number of graduate students, postdocs and undergraduate students, and his early results have led to substantial external funding, including single investigator NSF grants and a NYSTAR James D. Watson Investigator award, as well as considerable funding from the Department of Energy and the NIH. Todd also received the Dreyfus Teacher-Scholar Award and recognition as a Sloan Fellow. Work by Krauss and his group has resulted in independent publications including recent papers in high impact journals such as *JACS*, *Phys Rev. Lett.*, *Proc. Natl. Acad. Sci.*, *Science*, and *Nature*. He currently advises a large group comprised of twelve graduate students, three postdoctoral research fellows, and two undergraduates.

# Carolyn Bertozzi selected for 2009 Harrison Howe Award

The Harrison Howe Award of the Rochester Section of the American Chemical Society was presented to Professor Carolyn Bertozzi on October 1, 2009 at the University of Rochester. The event is an annual highlight of the local chemistry community that commemorates ACS Rochester Section cofounder Harrison E. Howe by recognizing a prominent scientist who has made outstanding contributions in chemistry, as well as demonstrated potential for further achievement. Prof. Patrick Holland was chair of the Harrison Howe Award Committee and Prof. Todd Krauss serves as one of its ten committee members. Valuable organizational assistance came from Debra Haring and Terri Clark.

Prof. Bertozzi, the T. Z. and Irmgard Chu Distinguished Professor of Chemistry and Professor of Molecular and Cell Biology at the University of California - Berkeley, is recognized as one of the leading scientists of her generation. Her research interests lie at the intersection of chemistry and biology, with a particular focus on understanding the relationship of cell surface glycosylation to normal cell function, and to human disease. Bertozzi has designed elegant experiments that have made historic contributions to the way in which researchers can profile changes in cell surface glycosylation associated with cancer, inflammation, and bacterial infection. She is most noted for her work in pioneering the field of bioorthogonal chemistry on living systems. She is also the director of the Molecular Foundry at the Lawrence Berkeley Laboratory.

*Patrick Holland presenting the 2009 Harrison Howe Award to Carolyn Bertozzi*



The Chemistry Department was pleased to host Prof. Bertozzi throughout her busy visit to Rochester, which also included many meetings with faculty in Chemistry, Chemical Engineering, Biophysics, and Biochemistry. She met with local graduate and undergraduate students from the Rochester area. She gave two energetic and inspiring lectures. The first was entitled “Imaging the Glycome with Bioorthogonal Chemistry,” an enthralling and well-attended talk that described her work on glycosylation. The evening award presentation featured a chemical biology themed poster session, and a lecture by Bertozzi describing the Molecular Foundry. This is a DOE-funded facility for synthesis of novel nanostructures and nanomaterials, where visitors can have access to sophisticated instrumentation and expertise.

With the 2009 award, Bertozzi joins a distinguished list of renowned chemists who have received this prestigious award since 1946. This is the highest award offered by the Rochester Section of the American Chemical Society, and particularly favors younger chemists who show promise for continued outstanding achievements. Approximately 40% of past Harrison Howe awardees have gone on to win a Nobel Prize. As of this past year, this list includes Jack Szostak, who shared the 2009 Nobel Prize in Physiology or Medicine after receiving the Harrison Howe Award in 2003.

*The 2009 Harrison Howe Reception and Poster Session, Sarah Flaum Atrium, URCM*



## David W. McCamant receives NSF CAREER Award



David W. McCamant, Assistant Professor of Chemistry received an NSF CAREER Award in July of 2009. The Experimental Physical Chemistry Program will support Prof. McCamant's research, which focuses

on ultrafast vibrational dynamics probed by femtosecond stimulated Raman spectroscopy, over the next five years.

The Faculty Early Career Development (CAREER) Program is a Foundation-wide activity that offers the National Science Foundation's most prestigious awards in support of the early career-development activities of those teachers-scholars who most effectively integrate research and education within the context of the mission of their organization. The activities build a firm foundation for a lifetime of integrated contributions to research and education.

In this project, the McCamant group will develop femtosecond stimulated Raman spectroscopy (FSRS) to study ultrafast processes in photochemistry and photobiology. The ultrafast dynamics of nucleic acids and short DNA oligomers will be investigated, as well as vibrational anharmonicities that drive vibrational relaxation in simple solvent models. Graduate students, postdoctoral scientists and undergraduate researchers will be trained in a wide variety of experimental and theoretical techniques throughout the funding period.

## A Date in History for Nuclear Science at the University of Rochester

For the first time, nuclear science has been introduced into the undergraduate curriculum at the University of Rochester. A new course has been developed in conjunction with the Physics Department entitled ANSEL - "Advanced Nuclear Science Educational Laboratory". The inaugural class was held in the spring of 2010 with undergraduate and graduate students from Chemistry, Physics, and the Laboratory for Laser Energetics.

Students enrolled in ANSEL will develop a sophisticated understanding of our terrestrial radiation environment and of some of the important applications of nuclear science and technology. They will acquire practical skills in the routine use of radiation detectors, monitors, and electronics, and develop the ability to assess radiation threats and prospects of their abatement. The four in-depth ANSEL experiments are designed to help students develop competence in the utilization of radiation detectors and analytical methods. The course should enable them to analyze experimental problems, to set



up nuclear instrumentation, and to conduct and analyze appropriate measurements. ANSEL, funded by a grant from the Nuclear Regulatory Commission and the Department of Energy, through provision of equipment and manpower, is taught by Udo Schröder, Prof. of Chemistry and Physics, with Frank Wolfs, Prof. of Physics. The DOE mission has profited

through the new training opportunities that have already been used by some graduate, undergraduate and Rochester high school students, who have participated in the setup and tests of the ANSEL experiments.

# Chemistry Welcomes Oleg Prezhdo

## Oleg Prezhdo

Professor of Chemistry

Ph.D. 1996, California Institute of Technology



### RESEARCH INTERESTS

Theory and modeling of quantum-classical dynamics of condensed phase chemical, physical and biological systems.

### CONTACT

prezhdo@chem.rochester.edu

Oleg Prezhdo was born in Kharkov, Ukraine in 1970. He obtained his Diploma in Theoretical Chemistry with Honors from Kharkov National University in 1991. His thesis work was on

many-body electronic structure theory and electron-vibrational dynamics under Prof. Anatoly Luzanov. From 1991 to 1993, he developed a continuum model of molecular solvation with Prof. Stanislav Tyurin in Kharkov Polytechnic University. Having moved to USA in the fall of 1993, he completed his Ph.D. on “Quantum-classical approaches for simulation of non-adiabatic chemical dynamics in solution” under Peter Rossky at UT-Austin in 1997. After a brief postdoctoral fellowship with John Tully at Yale, where he worked on constrained density-functional theory for electron transfer, he moved to the University of Washington in Seattle in 1998. In 2002, he was promoted to Associate Professor and in 2005 to Full Professor.

In 2008 Oleg became a Senior Editor of the *Journal of Physical Chemistry* and in 2010, was offered and accepted a Senior Professorship position here at the University of Rochester. Prof. Prezhdo’s research interests range from the fundamental aspects of semiclassical and non-adiabatic dynamics, to time-domain density functional theory, to photoexcitations in quantum dots, carbon nanotubes and molecule-bulk interfaces, to order-disorder transitions in electro-optic polymers and to the biological catch-bond.

Oleg is married to Marina Prezhdo and they have two children, Eugenia, 19, and Natalie, who is 6! They arrived on campus in August and we look forward to getting to know the entire family.

### Selected Publications:

Photoinduced dynamics in semiconductor quantum-dots: insights from time-domain *ab initio* studies. O. V. Prezhdo, *Acc. Chem. Res.* **2009**, *42*, 2005.

Theoretical aspects of the biological catch-bond. O. V. Prezhdo and Y. V. Pereverzev, *Acc. Chem. Res.* **2009**, *42*, 693.

Photoinduced electron dynamics at semiconductor interfaces: a time-domain *ab initio* perspective. O. V. Prezhdo, W. R. Duncan, and V. V. Prezhdo, *Prog. Surf. Science* **2009**, *84*, 39.

Breaking the phonon bottleneck in PbSe and CdSe quantum dots: time-domain density functional theory of charge carrier relaxation. S. V. Kilina, D. S. Kilin, and O. V. Prezhdo, *ACS-Nano* **2009**, *3*, 93.

*Ab initio* nonadiabatic molecular dynamics of wet-electrons on the TiO<sub>2</sub> surface. S. A. Fischer, W. R. Duncan, and O. V. Prezhdo, *J. Am. Chem. Soc.* **2009**, *131*, 15483.

Uniform diffusion of acetonitrile inside carbon nanotubes favors supercapacitor performance. O. N. Kalugin, V. V. Chaban, V. V. Loskutov, and O. V. Prezhdo, *Nano Lett.* **2008**, *8*, 2126.

Nonradiative quenching of fluorescence in a semiconducting carbon nanotube: a time-domain *ab initio* study. B. F. Habenicht, and O. V. Prezhdo, *Phys. Rev. Lett.* **2008**, *100*, 197402.

## Todd Krauss speaks at TEDx Rochester 2009



Professor Todd D. Krauss, Professor of Chemistry and Optics was one of the featured speakers at TEDx Rochester, a city-wide event to celebrate local “ideas worth spreading” held this past November, 2009. The day-long conference featured presentations of local thinkers, video broadcasts of speakers from around the world, performances by regional artists, and hands-on demonstrations of some of the city’s cultural institutions, packing Geva Theater with more than 450 guests (over 100 guests were turned away due to lack of space). The audience had the unique opportunity to hear and meet with innovators from area universities, museums and arts groups.

Prof. Krauss spoke on nanoscience and nanotechnology, the study and application of materials and integrated materials systems that have sizes approximately one billionth of a meter (one nanometer). A general overview of the field was presented, as well as why the nanometer scale size and shape are so important in determining the physical characteristics of particular materials. Several examples of commercial products containing nanometer scale materials already in the marketplace were discussed, in addition to areas where the potential for truly groundbreaking new technology from nanomaterials could be exploited in the future. In particular, nanomaterials science and technology are poised to someday be instrumental in powering the planet with clean, renewable, energy sources.

Finally, concerns about the safety and environmental effects of nanometer scale materials were also discussed.

TED, an international series of nonprofit symposiums launched in 1984, is an annual event where some of the world’s leading “thinkers and doers” are invited to share their passion for their fields. “TED” stands for Technology, Entertainment, Design — three broad subject areas considered to collectively be shaping our future. Rochester was one of 30 American cities hosting conferences by TEDx this year, a new offshoot of TED. TEDx events are independently organized in host cities and Rochester’s conference was sponsored by local businesses and foundations to highlight our city and its young, creative, and talented population.

### TEDx Talk Abstract

Nanoscience and nanotechnology is the study and application of materials and integrated materials systems that have sizes approximately one billionth of a meter, or one nanometer. One nanometer is about 100,000 times smaller than the width of a human hair, so these highly engineered materials and integrated systems are extremely tiny, similar to the size of proteins inside our cells. Nanomaterials exhibit the remarkable property that their basic physical properties such as color are often highly tunable by simply controlling the size and shape of the material, an effect fundamentally due to quantum mechanics. For macroscopic objects, tuning the color (say of a piece of metal) by changing its size or shape is just simply not possible. However, at the nanometer scale, the rules governing the physical properties of materials and how materials interact are different than for larger objects, thus enabling extraordinary and often unexpected behavior. Of interest to the scientific community for over two decades, the unique characteristics of nanomaterials and assemblies containing these materials has led to many inside and outside the field to see the potential for truly groundbreaking applications in numerous areas from biotechnology to renewable and sustainable energy. On the other hand, nanometer scale materials have also created concerns in the general public about their toxicity, overall environmental impact, and whether they will move beyond the relatively pedestrian commercial products currently available and truly live up to their potential.

# The 2010 Biological Chemistry Cluster Retreat

This year, the Biological Chemistry Cluster organized a Chemistry-Biology-Biophysics Interface Retreat, which was held on June 9th and 10th. The goal of the Retreat was to increase interactions between groups doing Biology, Chemistry, and Biophysics at the University of Rochester. The Retreat was funded by Provost Ralph Kuncl as a function of the University Committee for Interdisciplinary Studies (UCIS), which is chaired by Dave Goldfarb from the Biology Department. Prof. Harry Stern arranged the schedule and many members of the Cluster contributed to its success. Undergraduate Coordinator, Terri Clark, made sure that all ran smoothly, which allowed the participants to focus on science.

The Retreat started on the afternoon of June 9th with two talks given to an audience of about one hundred in the Class of '62 Auditorium in the Medical Center. The first talk was on "The unique properties of omega-3 fatty acids: implications for rhodopsin function" by Scott Feller, Prof. of Chemistry at Wabash College. The second talk was titled "On the species specificity of ribosomal antibiotics" by Peter Moore, Sterling Professor of Chemistry at Yale University. The latter lecture was the first Vincent du Vigneaud Lecture and was followed by a reception with wonderful food! Dr. du Vigneaud received his Ph.D. from Rochester's Biochemistry Department and went on to win a Nobel Prize. His daughter funded the du Vigneaud Lecture and reception in his honor.

The Retreat reconvened in the Meliora Restaurant on the River Campus at 9 AM the next day with 100 attendees. The day started with fruit, juice and bagels and a session of 19 posters ranging from synthesis to computations, with a wide variety of studies in between. This was followed by a very informative "Career Panel Discussion," that included Peter Moore, Scott Feller, Cary Bauer, Ph.D., from Bruker AXS, and Anne Schneiderman, Ph.D., Esq., of the law firm Marjama, Muldoon, Blasiak & Sullivan, LLP. As usual, common themes of the discussion were that careers rarely go in a direct line and that it helps to be lucky. The discussants gave

interesting and candid answers to questions and inspired the audience to think about their own career plans. This was facilitated by the buffet lunch which followed.

The afternoon program included six scientific talks from members of UR labs. Dr. Danna Eickbush (Department of Biology) presented her research on "R2 retrotransposons encode a self-cleaving ribozyme for processing from an rRNA co-transcript"; Dr. Andrea Lee (Krauss/Bren groups, Department of Chemistry) discussed "Using Zn(II) porphyrin fluorescence in FRET studies of cytochrome c folding"; Prof. Harry Stern (Department of Chemistry) brought us "Computational estimation of protein-ligand binding affinities;" followed by Jessica Smith (Fasan group, Department of Chemistry) on "Synthesis of macrocyclic organo-peptide hybrids from genetically encoded precursors"; Krystle McLaughlin (Kielkopf group, Department of Biochemistry and Biophysics) presented "Mechanism of NADH/NAD<sup>+</sup> sensing by the redox sensing repressor Rex"; and our last speaker, Joanna Touger Olsen (Dewhurst group, Dept. of Microbiology and Immunology) spoke on the topic "Do cationic amyloid fibrils present in semen enhance HIV-1 transmission?" This year's Retreat included posters and speakers from the Departments of Biochemistry and Biophysics, Biology, Chemistry, Microbiology and Immunology, and Pediatrics.

Much information was exchanged throughout the two days and new connections were made that can enhance interactions of chemists, biologists, and biophysicists at UR. Several attendees were undergraduates participating in the Department's summer Research Experience for Undergraduates program, which Tom Krugh directs. The Retreat provided them and all participants a broad overview of biological chemistry research at UR. The breadth represented is a particular strength of UR and stems from George Eastman's vision that the College should be adjacent to the Medical Center in order to facilitate interactions.

*Scott Feller, Harry Stern, Doug Turner, Peter Moore, Alan Grossfield, Kara Bren, and Joseph Wedekind (left to right)*



# Student Awards and Accolades

See also Commencement Awards on p. 58.



**MATTHEW GOLDER (B.S. '10)**, received the Ayman-Amin Salem Award which is awarded each year by the University to that member of the senior class who best evidences the qualities of good character and good citizenship, such as decency, reliability, responsibility and congeniality.

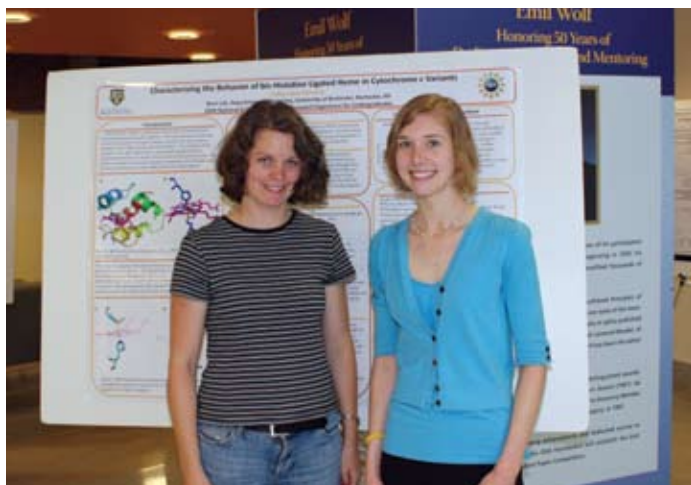
Ayman was a student in the Class of '87 who died in a car accident, the fund being established by his family in his memory. Matthew, who is attending graduate school this fall at Boston University, also received the 2010 ACS Rochester Section Award for his outstanding academic record. Matthew presented his research, under the direction of Patrick L. Holland, at the annual section meeting this past April.

**CAITLYN ROSE KENNEDY**, a senior B.S. chemistry and B.A. biology major, was awarded the 2010 Gladys Anderson Emerson Scholarship. This scholarship, funded by Iota Sigma Pi, is given to a woman in her third year of undergraduate studies for excellence in chemistry or biochemistry. Caitlyn has already received the Chemistry Department Freshman Achievement award, been elected to Phi Beta Kappa, and has been an outstanding teaching assistant for the past two years. Nominated by Professor

Bren, Caitlyn's impressive application, resume, essay, and letters of recommendation allowed her to be one of two students nationally to receive this award. In addition, Caitlyn received the 2010 Catherine Block Memorial Fund Prize, established in memory of Catherine Block, an exceptional Chemistry student here at the University. This prize is awarded each year to a woman in the Junior class in recognition of her outstanding ability and achievement in the field of science.

The 2010 University of Rochester Undergraduate Research Symposium was held this past April in which five Chemistry majors participated: **COLIN KINZ-THOMPSON (B.S. '10)**, and **RANDY MEHLENBACHER (B.S. '10)** both gave oral presentations and **BRIAN LINDLEY (B.S. '10)**, **MATTHEW GOLDER (B.S. '10)**, and **JULIE TABROFF (B.A. '10)** presented posters. The Symposium included participants selected by judges, reflecting the most accomplished undergraduate work throughout the College. Four sessions were running concurrently in separate locations on campus representing the four distinct disciplinary sections of the College: Humanities, Natural Sciences, Social Sciences, and Engineering. The Poster Presentation Fair served as a place for all undergraduate students who conducted research in the 2009-2010 academic year to present their findings to the College community. Colin Kinz-Thompson received the President's Prize, awarded to the top presenter in each discipline for his presentation on "Proton Transfer in the Adenine-Thymine Radical Cation Embedded in B-form DNA" under the mentorship of Prof. Esther Conwell. The research results were published in *J. Phys. Chem. Lett.* Colin, who is

*Kara Bren and Caitlyn Kennedy*



*Colin Kinz-Thompson*





attending Columbia University graduate school this fall, also received the John McCreary Memorial Prize and was elected to Phi Beta Kappa. Brian and Julie both received a Professor's Choice award for their posters (Advisors: Professor Richard Eisenberg and Professor Melanie Wellington, respectively). Brian, also elected to Phi Beta Kappa, received the 2010 ACS Inorganic Chemistry Award and a Carl A. Whiteman Teaching Award. This fall he began graduate school at Cornell University.



The recipients of the 2009 Iota Book Award included two undergraduate chemistry majors, **MARK LEVIN** (Edwardsville, IL) and **EMILY REDMAN** (Webster, NY). The University of Rochester's Iota Chapter of Phi Beta Kappa (the University's oldest honor society), along with deans of the College of Arts, Sciences, and Engineering,

recognized the winners during a formal ceremony this past December. Nineteen sophomores, among a class of more than 1,000 students, were recognized for their scholarly achievement, demonstration of humanistic values, and involvement in co-curricular activities during their first year at Rochester. In addition to evaluating academic records, the award committee collected nominations from professors, administrators, and College staff members. "This is an amazing group of students," said Edward Brown, president of the Iota Chapter of Phi Beta Kappa and assistant professor in the Department of Biomedical Engineering. "Their ability to make major contributions to the campus and the community while achieving the highest level of scholarship is truly inspiring." Emily has already received a Freshman Chemistry Achievement Award and both Emily and Mark have received a MERCK Index award. Both have also been teaching assistants for the department.



*Randy Mehlenbacher*

**RANDY MEHLENBACHER (B.S. '10)** was awarded the Wendy Jill Fread Prize, established in memory of Wendy Jill Fread, Class of 1975. This is presented by the University to the member of the senior class who, during four years as a student, has given the greatest service and shown the greatest concern for fellow students. In addition, Randy, a Phi Beta Kappa double chemistry and physics major, received the Dr. E.W. and Maude V. Flagg Award from the Chemistry Department and the Stoddard Prize from the Physics Department. Randy was an excellent teaching assistant during his undergraduate years here and he conducted research in Dave McCaman's lab. He started in the graduate program at the University of Wisconsin this fall.

Each year, the University awards the Janet Howell Clark Prize to the senior woman who has shown the greatest promise in creative work in Physics, Chemistry, Biology, or Astronomy, and who has shown outstanding versatility in the mastery of allied fields. This year, chemistry and biochemistry double major **JULIE TABROFF (B.A. '10)** received the JHC Prize, as well as a chemistry department senior award. Elected to Phi Beta Kappa, Julie was also an outstanding teaching assistant for both chemistry and biology and received a Carl A. Whiteman Jr. Teaching Award at Commencement. Julie is now attending the University of Massachusetts Medical School to pursue a career in pediatric medicine.



*continued on next page* 



Chemistry third-year graduate student, **MEGHAN CLARK** (Holland group) received The Edward Peck Curtis Award for Excellence in Teaching by a Graduate Student. This award is given to exceptional teaching assistants selected in a University-wide competition. The

nomination is comprised of letters of support from the Chair, faculty, and students. The recipients are honored at a luncheon with the Provost and Dean of Graduate Studies. Recent winners have also been Chemistry students: Wesley Asher, Mary Lenczewski, Amy Ensign, Lisa Carlson, and Jerry Manbeck.

**DANIEL EVERSON**, a second-year graduate student in the Weix group, was awarded an NSF Graduate Research Fellowship. The National Science Foundation (NSF) offers fellowships to students in their early stages of pursuing research based Master's or Ph.D. degrees. In addition, **KENNETH LOTITO (B.S. '08)** and **KATIE KNOWLES (B.S. '08)** won NSF Graduate Research Fellowships with Katie also a recipient of a DOE Fellowship. Kenny started out in the graduate program at MIT but transferred with his adviser, Jonas Peters, to CalTech. Katie is in the Weiss group at Northwestern University. Both Katie and Kenny worked with Prof. Rich Eisenberg in the 2006 REU program. **RANDY MEHLENBACHER (B.S. '10)** received an Honorable Mention from the NSF.



Meagan Evans



**MEAGAN EVANS**, a fourth-year graduate student in the Jones Group, received an ACS Division of Inorganic Chemistry Student Travel Award. She attended the ACS National Meeting in San Francisco from March 21-25, 2010, to present "Energetics of C-H Bond Activation Using [Tp<sup>+</sup>Rh(CNneopentyl)]: Quantifying Resonance Stabilization." Meagan co-authored a cover article (award) for the *Journal of Organic Chemistry* in 2009: "Thermodynamic trends in carbon-hydrogen bond activation in nitriles and chloroalkanes at rhodium." Meagan also received a Dean's



International Travel Award and recently returned from the 24th Annual International Conference on Organometallic Chemistry in Taiwan to present her research. She was joined there by **KAREN CHIANG**, a fourth-year graduate student in the Holland Group, who was a second recipient of a Dean's International Travel Award. Karen presented her research on binding to three-coordinate iron complexes, which has been published in *Inorganic Chemistry*.

**MATTHEW LIPTAK**, a postdoctoral fellow in the Bren lab, was awarded a continuation (competing renewal) of his National Institutes of Health Ruth L. Kirschstein National Research Service Award Individual Fellowship. The award is based on his proposal entitled "NMR and DFT Investigation of Porphyrin Conformation in Cytochromes c" and provides funding through May of 2011. Prior to joining the Bren group in the Department of Chemistry, Matt received his B.A. in 2003 at Hamilton College and earned his Ph.D. at the University of Wisconsin-Madison under the direction of Thomas C. Brunold in 2008. In his postdoctoral research, Matt integrates his past training in computational chemistry and physical inorganic chemistry with developing skills in NMR of paramagnetic biomolecules to gain a deeper understanding of factors that determine paramagnetic shifts of heme nuclei in proteins.



**CHRISTOPHER EVANS** (Krauss group) was selected to attend the Advanced Studies Institute on Nanomaterials and Nanocatalysis for Energy Applications between March 27 – April 5, 2010 in Cairo, Egypt. Sponsored by the US



Chris Evans



Lisa Carlson

National Science Foundation, the conference showcased an interdisciplinary cast of professors and student researchers from both the US and Egypt which highlighted current and future uses for nanomaterials. A cultural program fostered US-Egyptian relations with group tours to many of the regions notable historical monuments and musuems.

Each year, the University establishes award committees comprised of faculty members to determine the winners of the Outstanding Dissertation Award. This past academic year, **LISA CARLSON (PH.D. '09)** from the Krauss lab, was one of the three top winners for her thesis on "Photophysics of individual single-walled carbon nanotubes". Lisa, who defended in the fall of 2009, has taken a faculty position at Southern Connecticut State University.

year graduate student, also from Eisenberg's lab, received an ACS Division of Inorganic Chemistry Travel Award to attend the fall 2010 ACS meeting in Boston, MA.

This past year was a successful one for *Hutch's Hitters*, the UR Chemistry Department softball team. Teams are organized by fourteen different departments from the River Campus and UR Medical Center. The Chemistry Department team is comprised of faculty, and graduate students and their spouses. Strong hitting by rookie **MIKE PRINSELL** (.742) and veteran **JIM HART** (30 RBI) helped the team to finish the regular season with a record of 7-2, earning them a #2 seed in the playoffs. Led by solid defense from infielders **BRIAN OHMAN** (3B) and **ERIC HENRY** (SS), outfielders **TODD KRAUSS** (LF) and **DAN EVERSON** (CF), and phenomenal pitching by **BOB BOECKMAN**, they capped off a magical playoff run by defeating OsteoFerocious 5-3, and the BoMbErs 5-4 to win their first championship in recent memory. The coach, **MATT BETUSH**, would like to thank former coach **KATIE SEIFERT LEACH (PH.D. '09)** and the entire team for their hard work and determination.



**TULAZA VAIDYA**, a third year graduate student in the Eisenberg and Frontier groups, was featured in a *Nature Chemistry* article, "Iridium catalysis: try the trication." **JERRY MANBECK**, a fourth-

**2009 Hutch's Hitters (left to right):**

Mike Prinsell, George Arab, Brian Ohman, Michelle Wrubel Ryan, Derek Ryan, Rory Cottrell, Todd Krauss, Matt Betush, Jim Hart, Kendra Ohman, Pat Holland, Ria Swanekamp, Dan Everson, Bob Boeckman, Justin Rhinehart, Eric Henry



## Robert K. Boeckman, Jr.

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

Ph.D. 1971, Brandeis University



### RESEARCH INTERESTS

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

### CONTACT

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During the 2009-2010 academic year, **ROBERT K. BOECKMAN, JR.** completed his seventh year as the Chair of the Chemistry Department. Professor Boeckman is continuing as Chair for the 2nd year of a 3-year term in 2010-2011. 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 that 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  $\alpha$  oxidation of aldehydes and other applications. A new collaborative project has been initiated with Prof. David Goldfarb of the Biology Department whose goal is 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.

**NATHAN GENUNG (PH.D. '10)** defended his thesis in December 2009, and moved to UC Irvine, where he began

work as a postdoctoral associate in Larry Overman's group. **XINYI SONG (PH.D. '07)** continues as a senior postdoctoral fellow at Scripps in Florida working under Ted Kameneka and Bill Roush. **KE CHEN (PH.D. '07)** and her spouse **SAM ZHANG (M.S. '04)** are employed in New Jersey at BMS and Provid respectively. Other recent graduates of the group, **DAVID MIN (M.S. '06)** and **PHILIP WARBURTON (M.S. '06)** are pursuing employment as chemists in industry. **YAN MILLER (PH.D. '10)**, **JOHN MILLER (PH.D. '10)**, and Matt Betush continued their research in the group all on various aspects of asymmetric catalysis. Yan and John were married in September and defended their theses in March before moving on to postdoc's with Barry Trost at Stanford. George Arab and Brian Ohman delivered their third year seminar and continue working on FK-506 and Apoptolidin, respectively. Part-time scientist Dr. Dennis Savage, retired from Kodak, continues his work in the group on several projects with industrial collaborators. **REBECCA MURPHY (B.S. '09)**, who worked with the group during the 2008-2009 academic year as an undergraduate, just completed her first year of Ph.D. studies in Chemistry at UC Berkeley. Another former undergraduate group member, **JOHN BERTOLA (B.A. '09, M.S. '10W)**, has completed a Masters degree in Education at the UR Warner School and is working here at the UR this year with plans to eventually teach chemistry at the high school level, hopefully in the Rochester area. In the summer '09, three undergraduates worked in the group as part of the NSF REU program: Toby Maxwell from SUNY Geneseo; Doug Tusch from RIT, where he works with Boeckman group alumnus **JEREMY CODY (PH.D. '04)**; and David Kaphan, a rising sophomore. Doug began graduate school in the Department in the Fall 2010. David, who spent this summer as an intern at Novartis in Cambridge, MA, Emily Hart, who spent her summer doing research in Germany at Heidelberg U., and senior Chris Wong are working in the group during the 2010-2011 academic year.

## Kara L. Bren

Professor of Chemistry

Ph.D. 1996, California Institute of Technology



### RESEARCH INTERESTS

Bioinorganic and biophysical chemistry: heme proteins, protein folding and dynamics, NMR of paramagnetic biomolecule, solar energy conversion

### CONTACT

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The **KARA BREN** group is continuing its studies of structure, function, folding, and dynamics of heme proteins. The group celebrated the successful thesis defense by **AMY ENSIGN (PH.D. '09)** who was jointly advised by Todd Krauss. Amy was the brave pioneer of the protein folding project and is now starting her own adventure as an Assistant Professor of Chemistry at Roberts Wesleyan University in Rochester. Postdoc Andrea Lee and graduate student Wesley Asher are developing studies of protein folding on the single-molecule level. Andrea had a nice communication appear in the *Journal of the American Chemical Society (JACS)* reporting her work, and Wes filed a patent on a new method he developed in the course of the project to use “heme tags” for protein purification and quantitation.

The long-running project in the group is the study of relationships between structure and function in heme proteins using NMR, with an emphasis on analysis of chemical shifts in paramagnetic systems. Sarah Bowman completed her work on this project and defended her thesis in August 2010, after which she moved to Boston for a postdoc at MIT with Profs. Cathy Drennan and Collin Stultz. Postdoc Matt Liptak recently published a manuscript in *JACS* reporting relationships between heme chemical shifts and heme ruffling. Matt also commenced a collaboration with Liz Ledgerwood and Sigurd Wilbanks at the University of Otago (New Zealand) to examine electronic structure and electron transfer activity in human cytochrome *c* mutants associated with altered cell death (apoptosis). Graduate student Mehmet Can has been busy identifying novel relationships between NMR and EPR data on heme proteins in collaboration with Kristoffer Andersson's group at the University of Oslo, while also working on a crystal structure with the assistance of Prof. Joe Wedekind and Dr. Jermaine Jenkins. Third-year graduate student Jesse Kleingardner has been developing resonance Raman as a tool for this project while also pursuing NMR studies of some novel mutants of mitochondrial cytochrome *c*. The group was pleased to welcome first-year student Huixi “Violet” Zhang on this project who is commencing

heteronuclear NMR studies of heme and its ligands.

A major addition for the group was a new project funded by the DOE, “Modular nanoscale and biomimetic assemblies for photocatalytic hydrogen generation” along with Co-PIs Rich Eisenberg, Pat Holland, and Todd Krauss. First-year student Lenore Kubie, who is jointly advised by Todd Krauss, is bringing her experience with porphyrins and nanotubes to this project, and graduate student Erin Knappen brought her experience in protein engineering to the team.

Kara has had a busy year managing three projects in the lab and serving as Chair of the Bioinorganic Subdivision of the Division of Inorganic Chemistry of the American Chemical Society. She also traveled to give talks at universities and conferences, with a highlight being the International Conference on Biological Inorganic Chemistry in Nagoya, Japan.

*The former home of Chemistry, Lattimore Hall*



# 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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Last year the **CONWELL** group began simulations to obtain the wavefunction of a hole on a DNA duplex with one chain consisting of 10 adenines (A's) and the other chain 10 thymines (T's), both attached to the usual backbone of sugars and phosphates and surrounded by water. The code used was CP2K, set up especially to treat molecules with an open shell. The calculations use molecular dynamics to introduce the thermal motions of the atoms, and quantum mechanics to determine the resulting wavefunctions and energies. CP2K is available in the literature but with little documentation; setting it up to carry out a simulation requires a great deal of computer knowledge and work. The work was carried out over a period of about a year by an undergraduate, **COLIN KINZ-THOMPSON (B.S. '10)**. He then carried out two simulations for initial temperatures of 20K and 300K, respectively. The temperatures were not kept constant, however, but allowed to rise during the simulations. The results of the simulations had some surprises. Immediately after introduction of the hole it was found to be spread over 5 adenines (the extent of the region in which quantum mechanics was used to determine the wavefunction) with very little on the thymines, as expected. For both the "20K" and the "300K" runs the extended wavefunction starts to contract as soon as the hole is introduced. By  $\sim 20$  to 25 fs the wavefunction is localized on one A, with small amplitude on each of the neighboring A's. It remains contracted for the duration of the runs, a few hundred fs. For the "20K" case, at about the time the contraction is complete the proton at the adenine end (N6) of one of the hydrogen bonds to thymine begins to move toward the other end of that hydrogen bond (O6) at thymine. By a little less than 60 fs proton transfer from A to T is complete. At that time the temperature is  $\sim 180$ K. The proton stays transferred to the end of the run, where the temperature is  $\sim 220$ K. For the "300K" run no proton transfer is seen. The results of

the "20K" run are of particular interest because it had been predicted by Steenken, on the basis of pKa measurements, that proton transfer would not take place in A:T. There are, as yet, no experimental results showing proton transfer in A:T. Our work was published in *J. Phys. Chem. Letters*. We will be looking into the reasons for the contraction and the proton transfer.



*Esther Conwell with Colin Kinz-Thompson*



## RESEARCH INTERESTS

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

## CONTACT

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**JOE DINNOCENZO** and his group continue to pursue a variety of problems in photoinduced electron transfer and related chemistry. In one project we discovered that ground state electron transfers between neutrals and cation radicals have a rate constant/driving force dependence that surprisingly follows a simple Boltzmann type behavior. We also found that the charge shift, electron transfer quenching of excited pyrylium cations by neutral donors also had a Boltzmann dependence. Most surprisingly, we found that excited state quenching of neutral cyanoaromatics by neutral electron donors had a Boltzmann dependence on the driving force for electron transfer. Our results contrast with the well-known Rehm-Weller description of excited state electron transfer quenching ( $k_q$ ) involving neutral donors and acceptors ( $A^* + D \rightarrow A^{\cdot-} + D^{\cdot+}$ ), where a gradual fall off in  $\log k_q$  vs  $\Delta G$  is reported. This caused us to carefully re-examine all of the original Rehm Weller data. Remarkably, when accurate redox potentials are used for the electron donors and acceptors, and when one excludes data points in the highly endergonic region that are not due to electron transfer, the quenching rate constants for the experiments described by Rehm and Weller also follow a Boltzmann dependence on driving force! It seems likely that our work will lead to the reinterpretation of a large body of previously published data, which relied on the original Rehm Weller analysis and approach. We have also made significant progress this past year on understanding the unusual chemistry of aryltrimethylstannane cation radicals, which are unique amongst known Group 14 cation radicals in that they undergo  $S_N1$  C bond fragmentation to preferentially give the less stable aryl radical rather than a methyl radical. Our experiments show that the stannane cation radical fragmentations are *not* unimolecular, as previously thought, but are nucleophile assisted. This new reaction mechanism can readily explain the otherwise perplexing chemistry of these stannane cation radicals. The group also continues to investigate various aspects of the chemistry of organosilane and organogermane cation radicals.

On the teaching front, Joe had a good experience with the first year graduate students last fall in CHM 433 (Physical

Organic I). In the spring, Joe was on sabbatical, which gave him an opportunity to get into the lab and work with Samir Farid. Joe looks forward to teaching CHM 210 (Honors Organic Laboratory II) in the spring of 2011, when he will continue an experiment to introduce Peer Led Team Learning (aka Workshops) into the course. Joe will be working with Ms. Terrell Samoriski, who will assist in the design, implementation and evaluation of the workshop model as part of her Ph.D. research in chemical education.

As for group news, Mary Lenczewski is close to wrapping up her Ph.D. research on the stereochemistry of organo-silane and germane cation radical substitutions. Fourth-year graduate student Pu Luo has completed a project using stereochemical probes to test the reversibility of  $S_N2$  reactions on organosilane cation radicals and is making excellent progress on understanding the chemistry of stannane cation radicals. A new student – Gigi Criss – joined the group this spring and will start working on the chemistry of aryltrialkylsilane cation radicals. Terrell Samoriski also joined the group this past year. In a pioneering effort, she will be conducting educational research toward her Ph.D. in Chemistry. The group continues to benefit from a long standing collaboration with Dr. Samir Farid on a range of research projects.

*The Eastman Quadrangle and Schlegel Hall*



# Richard Eisenberg

Tracy H. Harris Professor of Chemistry

Ph.D. 1967, Columbia University



## RESEARCH INTERESTS

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

## CONTACT

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**RICH EISENBERG** writes: This has been a fantastic year - it doesn't get any better. In March I was called by Bruce Jacobs, Dean of Graduate Studies in The College to inform me that I would be recognized at graduation with the University Lifetime Achievement Award in Graduate Education. At the end of April, I received notification that I had been elected to the National Academy of Sciences, one of the highest honors to which we aspire in science. And then at graduation, listening to all the compliments and accolades was truly over the top. I won't say anyone was wrong in what they said but lots of salt would be needed for all of the comments, preferably around the rim of a large margarita glass. It was one of those times when everything goes right in the world. All of this comes after last October when I was inducted into the American Academy of Arts and Sciences in Cambridge, MA and signed the academy book that continues a tradition dating back to John Adams and the founding fathers. I was delighted my family were all there to see the happy event.

In my comments at the UR Graduate Degree Ceremony where the Lifetime Achievement Award was conferred, I thanked my family, my teachers, my colleagues and "my graduate students and postdoctoral researchers whom I have mentored and worked with over the years, the many undergraduates who have done research in my lab and allowed me to influence how they viewed chemistry, and finally the legions of undergraduates whom I have taught in general chemistry, inorganic chemistry and other courses. All of these folks have truly enriched my life." Students are a key reason teachers do what they do. I believe that not only have students enriched my life, they have made me younger in the process.

On the science front, our work on the photogeneration of H<sub>2</sub> from water - the reductive side of water splitting - has made strides forward with better mechanistic understanding and higher turnovers than before. In this light, we continue efforts to develop new robust, durable and highly active systems for H<sub>2</sub> generation. Research on this problem is spear-headed by postdoctoral researchers Theresa McCormick and Bill McNamara, as well as new 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 me for a multi-pronged approach

to the light-driven generation of hydrogen from water. I firmly believe solar energy conversion into stored chemical potential is the key to success in meeting the challenge of abundant energy for sustainable development.

We also made significant progress this year on iridium catalysis of electrocyclization reactions in a joint project with Alison Frontier that was carried forward by graduate student Tulaza Vaidya and postdoctoral researcher Jing Zhang. One of our studies was highlighted in *Nature-Chemistry*. New results were also obtained by graduate student Jerry Manbeck on luminescent Cu and bimetallic Cu/Au complexes, including one system that contains a steroid derivative as a ligand and is impressively bright in photoemission. Some possible applications of these luminescent complexes are being explored.

Group comings and going for the year include the arrival of postdoc Bill McNamara from Yale, first year graduate student Zhiji Han (as noted above, both co-advised with Pat Holland) and Randy Sabatini who will be co-advised with Dave McCamant. Departures included **JING ZHANG (POSTDOCTORAL FELLOW '10)**, who will be returning to China, and **MARCO CRESTANI (POSTDOCTORAL FELLOW '10)**, who moved to a postdoc position at Purdue, and visiting graduate student Geng-geng Luo from Xiamen University in China. The past year I also had three undergraduate researchers working in my lab, two of whom were moving forward to obtain their Master's degrees in a compressed schedule. The combined B.S./M.S. students were **ALEXANDER (SASHA) SOKOLSKY (B.S. '10)** who worked on iridium chemistry and **DAVID FARKAS (B.S. '10)** who conducted experiments on semiconductor surface modification for H<sub>2</sub> generation. The third was **BRIAN LINDLEY (B.S. '10)** who also conducted research on making H<sub>2</sub> with new organic dyes and soluble Co catalysts. Sasha is attending the University of Pennsylvania this fall and Brian is at Cornell, both in chemistry Ph.D. programs. David is now looking to commence an M.D./Ph.D. program, based in part on his interest nurtured during the past year of research. Finally, Prof. Gabriel Garcia-Herbosa from the University of Burgos in Spain began a 6-month sabbatical stay with us in April and is impressing all of us with his Spanish treats as well as his knowledge of chemistry.



*Inorganic Chemistry* continues to do well. The most recent Thomson Scientific Report of journal impact factors and citations shows *Inorganic Chemistry* to be at the top of its class with more than 79,450 citations and a record high impact factor of 4.657. I continue to be grateful for the tireless efforts put in by Arlene Bristol, Kirstin Campbell and spouse Marcia in the Editor-

in-Chief's office to keep the journal running so successfully. The changing scene in scientific publication is both stimulating and interesting as the electronic information age and now the smart device revolution continue. Attempting to figure out how scientists, particularly young ones, access and use information, and how they will disseminate their results in the future pose genuine challenges that I am happy to continue to address.

*The Eisenberg Group, Summer 2010*



## Samir Farid

Research Professor

Ph.D. 1967, Göttingen University



### RESEARCH INTERESTS

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

### CONTACT

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The focus of **SAMIR FARID**'s research continues to be on electron transfer reactions and kinetics. Reevaluation of the dependence of thermal and photochemical electron transfer rate constants on the reaction energetics was the main focus of this year's activity. This work has provided a different perspective that changes long-accepted ideas.



*Sunset over Fauver Stadium in the winter*

# 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

farrar@chem.rochester.edu

**JIM FARRAR**'s interest in crossed beam studies of low energy ion-molecule reactions continues, and with NSF support just awarded, he looks forward to beginning a new series of studies on ion-radical reactions using imaging techniques. New tricks for an old dog, as the saying goes around here!

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.

Three years ago, Jim introduced Peer-Led Team Learning (PLTL) workshops into the freshman chemistry lab, and the results of that activity are beginning to bear fruit. Students are becoming more engaged and excited about the freshman lab experience, and the teaching assistants are becoming partners with the students, helping them "think like scientists."

PLTL workshops are an integral component of all of Jim's teaching, in freshman chemistry and lab, and in physical chemistry. He has enjoyed working with many talented undergraduate and graduate students as workshop leaders, and has particularly enjoyed collaborating with Dr. Catherine Perez from the Learning Assistance Services office to help leaders become more effective mentors for their students. The large number of students in the course who volunteer to be workshop leaders is a strong testimony to the success of the program.



*Flowers in front of the University Bookstore*

# Rudi Fasan

Assistant Professor of Chemistry

Ph.D. 2005, University of Zürich, Switzerland



## RESEARCH INTERESTS

Bioorganic chemistry; enzyme engineering and directed evolution; chemo-enzymatic synthesis; chemical biology.

## CONTACT

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The research interests of the **FASAN** group gravitate around the design and development of chemo-enzymatic and chemo-biosynthetic methods to direct the assembly and functional diversification of biologically relevant organic skeletons. A major project of the group focuses on the implementation of P450-based methodologies for the functional elaboration of organic compounds via P450-mediated oxidation of aliphatic C-H bonds. Combining P450 catalysis, protein engineering, and chemical synthesis we aim at exploring and developing new synthetic routes for the selective functionalization of non-activated C-H bonds in complex molecules. During the past year, important progress has been made in this area thanks to the hard work of postdoc Kaidong Zhang and the help of UR undergraduate students Shady El Damaty and Tasha Raman who worked in the lab as part of an independent research course. An important milestone was reached by validating a novel P450 fingerprinting method for predicting the reactivity of engineered P450 variants. This opens the way to the development of systematic approaches to simplify the search of P450 catalysts with tailored activity, regio- and stereoselectivity towards target natural products. Another notable achievement consisted in the successful application of P450-mediated synthesis to afford unconventional functionalizations on the artemisinin scaffold, a naturally occurring sesquiterpene lactone with important antimalarial activity. Continuing efforts will explore the activity of these new semisynthetic artemisinin derivatives against *Plasmodium falciparum* through collaboration with the Morrell group at the UR Medical Center.

First-year graduate student John Frost and undergraduate students **JACQUELINE ZAENGLE (B.S. '10)** and Rajesh Ravikumar have also reported success in their collaborative efforts towards modulating the regio- and stereoselectivity properties of P450 enzymes using non-natural amino acids. After leaving for a study experience in Japan, Jacqueline will return to the lab in September to conduct senior research during the upcoming academic year as a Take 5 student. Rajesh has continued working in the group during the summer supported by a REU fellowship.

During the past year, we witnessed a breakthrough in our efforts towards the development of a chemo-biosynthetic strategy for generating macrocyclic organo-peptidic hybrids. Jessica Smith, Francesca Vitali, and Maragani Satyanarayana have been the key players in this project. We look forward to seeing how this strategy will enable the

'evolution' of small size chemical probes for targeting proteins and protein-protein interactions. Jessica Smith completed her second year oral exam in July and she continues to enjoy her support from the NSF Graduate Student Fellowship.

First-year graduate student Yekaterina (Katia) Lyubarskaya joined the group in January 2010 and began working on a method to produce self-cyclizing peptides in living bacteria. During the past summer, we enjoyed the presence of several undergraduate students who conducted research under the auspices of the REU and McNair program or volunteered to work in the lab to gain experience in synthetic chemistry and protein engineering. These include UR students Nicholas Jacob (REU), Soaiful Islam (McNair), Brian Shafer, and Jeongeun (Catherine) Kil, and REU fellow Kenneth Myers visiting from Bloomsburg University. We are grateful to them for their help to the group's ongoing projects and for contributing to making the lab atmosphere even more enjoyable. The summer experience culminated with a barbeque party (photo below) and a fierce competition across a ping pong table, from which Brian emerged as proud and unbeaten winner.

In Fall 2009, Rudi started teaching the undergraduate course 171Q (Quest Organic Chemistry I), in addition to the Bioorganic Chemistry and Chemical Biology (CHM 437) course. Teaching the larger class of freshmen was an exciting and rewarding experience and Rudi looks forward to repeating it during this academic year.

*Get-together of current and past members of the Fasan group, July 2010.*



# 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

frontier@chem.rochester.edu

Professor **ALISON FRONTIER**'s research program is devoted to the planning and execution of syntheses of biologically and structurally interesting natural products. The study of Nazarov cyclization continues, as more and more variations on the cyclization are uncovered. The development of rearrangement chemistry gets more and more interesting, as have efforts to discover alternative starting points for the  $4\pi$  electrocyclization. Work on asymmetric cyclizations and applications of Nazarov cyclization toward total synthesis of natural products continues. The study of diastereoselective hydrogenation of pyrroles is also underway, as well as efforts toward the synthesis of three terpenoid natural products, phomactin A, norcembrenolide and cyanthawigin.

Tulaza Vaidya (third-year student, working jointly with Rich Eisenberg) has developed remarkably active Ir(III) complexes as Nazarov cyclization catalysts. We continue to study rearrangement chemistry that occurs during Nazarov cyclization (Eric Theiste, third-year student; and Dr. David LeBoeuf). Two additional interesting versions of the Nazarov cyclization are also under investigation: Bill Spencer (second-year

student) is initiating Nazarov cyclization by oxidizing vinyl alkoxyallenes, a reaction we first implemented in the total synthesis of rocaglamide, and Josh Brooks (second-year student) is initiating Nazarov cyclization by adding nucleophiles to unsaturated diketones. All three of these variations give cyclopentane-containing products that are quite different from the cyclopentenone products of conventional Nazarov cyclization. Natural product news: Jen Ciesielski (third-year student) has made a series of interesting (and challenging) discoveries on the warpath pursuing phomactins A and D, allowing us to consider the intricacies of macrocycle architecture firsthand.

In the fall, three first-year graduate students joined the group. Peter Carlsen is pursuing total synthesis of the elusive tetrapetalone A, Steven Jacob will develop methodology for the synthesis of complex pyrrolidines via diastereoselective and enantioselective hydrogenation of pyrroles, and Yu-Wen Huang will pursue the efficient and enantioselective synthesis of roseophilin.

*Hutchison Plaza*



## 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

goodman@chem.rochester.edu

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



*Josh Goodman at the 2009 Commencement Ceremony*

## Patrick L. Holland

Associate Professor of Chemistry

Ph.D. 1997, University of California, Berkeley



### RESEARCH INTERESTS

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

### CONTACT

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**PATRICK HOLLAND** and his research group are going strong! They continue their research on the chemistry of iron- and cobalt-containing compounds, motivated by the catalytic chemistry of these metals in the environment, in biological systems, and for organic and inorganic synthesis. We are especially excited to have a new influx of grants to support our research. First, a grant from the National Science Foundation will support a project aimed at iron-imido complexes for stoichiometric and catalytic amination reactions. This is a collaboration with **BRIAN EDELBACH (PH.D. '99)**, a professor at Monroe Community College who is doing summer research on the project at Rochester with two of his students. Secondly, a grant from the Department of Energy aims to uncover new catalysis with low-

coordinate cobalt complexes. This grant was enabled by outstanding preliminary work from recent graduate **KEYING DING (PH.D. '09)**, which were published as two Communications in *Journal of the American Chemical Society*, one of which received special coverage in *Nature-Chemistry*. The DOE grant also enabled us to purchase a new X-band EPR spectrometer for analysis of paramagnetic compounds. Third, we have received renewed funding from the National Institutes of Health for our continuing work on reactions of dinitrogen ( $N_2$ ) as it relates to the enzyme nitrogenase. Finally, a joint grant with Profs. Bren, Krauss, and Eisenberg has opened the door to a new project on light-driven  $H_2$  production.

*continued on next page* 

The Holland group enjoys our collaborative work with a number of other researchers around the world, including the following: Timothy Machonkin (Whitman College) on an iron enzyme that degrades toxic waste; Eckhard Bill (Max-Planck-Institut für Bioorganische Chemie, Mülheim, Germany) on Mössbauer spectroscopy; Brian Hoffman (Northwestern) on EPR and ENDOR spectroscopy; Kent Rodgers (North Dakota State) on resonance Raman spectroscopy; Markus Ribbe (UC Irvine) and Lance Seefeldt (Utah State) on nitrogenase; Chaim Sukenik (Bar Ilan University, Israel) on surface attachment; Tom Cundari (North Texas) and Frank Neese (University of Bonn, Germany) on computations; and, Brian Crane (Cornell) and Serena DeBeer (Cornell) on X-ray techniques. Interacting with these leading researchers around the world is a super experience for students, and the expertise of our collaborators enables us to do the most thorough possible science.

Every year has its exciting arrivals and departures. We bid a fond farewell to **SARA ROCKS (PH.D. '09)**, who has moved to a postdoctoral position doing biogeochemistry with Francois Morel at Princeton University. Two undergraduate students graduated in May: **MATTHEW GOLDER (B.S. '10)**, who will be going on to Ph.D. work at Boston University, and **ETHAN KAPLAN (B.A. '10)**, who will be doing an internship in Israel. We have welcomed new group members Nicole Wedgwood (Masters student coming from Ithaca College), Aydin Kavara (postdoctoral fellow coming from U. Michigan), and Jonathan Goldberg (undergraduate student at UR). We were also joined by two joint Holland/Eisenberg students concentrating on H<sub>2</sub> production: first-year graduate student Zhiji Han (coming from UC-San Francisco) and postdoc Bill McNamara (coming from Yale).

*The Holland Group synthesizes ice cream  
Spring 2010*

This year, fourth-year student Ryan Cowley was the recipient of an Elon Hooker Fellowship that recognizes his research accomplishments. Ryan previously received an NSF Graduate Fellowship, and has been an exceptional researcher with six first-author papers in print or in progress. Ryan has also taken important leadership roles in the department including hosting Rothchild Lecturer Robert Crabtree, and co-initiating a new student ACS Meeting practice seminar series. Fourth-year student Karen Chiang received a DeRight Fellowship, in recognition of her great research. Karen is valued as a fixture in the organization of the graduate student recruiting weekend. Karen is also our most photogenic group member: she even appeared in a TV commercial last fall! Last but not least, third-year student Meghan Clark was recognized with a Curtis Teaching Award in recognition of her outstanding work with CHM 234 ("Advanced Synthetic Techniques"), as well as a Lattimore Fellowship in recognition of her research. These are just examples of the many efforts of all the great Holland group graduate students.

In addition to research, Pat took part in his usual mix of teaching graduate and undergraduate courses, traveling to conferences and invited lectures, and service to the chemistry community. In particular, Pat joined the Executive Committee of the ACS Division of Inorganic Chemistry as Awards Co-Chair. Last but not least, he was promoted to full Professor as of July 2010.

Alumni news: **BRYAN STUBBERT (POSTDOC. '07)** and his wife Rebecca welcomed baby Hazel into the world in March 2010. **TRAVIS HEBDEN (B.S. '04, M.S. '05)** moved to a postdoctoral position with Nobel Laureate Richard Schrock at MIT. **AZWANA SADIQUE (POSTDOC. '07)** is teaching at Monroe Community College and is living happily in Henrietta with Rezan, Anah and



# William D. Jones

Charles F. Houghton Professor of Chemistry

Ph.D. 1979, California Institute of Technology



## RESEARCH INTERESTS

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

## CONTACT

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The **JONES** group continues to actively pursue organometallic chemistry and catalysis. We had two new graduate students join the group this year, and one student graduated this winter. We have a new postdoc in the group, Dr. Sabuj Kundu from Rutgers University. We also have one new incoming graduate student in the lab this summer and the lab is at full capacity with 11 people. We are planning renovations for this fall that will expand the capacity to 13 people. Our research is examining the activation of C-H bonds in substituted hydrocarbons, the cleavage of carbon-carbon bonds in alkynes and nitriles, and the C-S cleavage/hydrogenation of thiophenes. These projects have involved a variety of fundamental studies of model reactions, as well as actual catalysis. We have established an important understanding on the factors that control metal-carbon bond strengths that allows us to make predictions about stabilities. The group continues its role in the Center for Enabling New Technologies through Catalysis (CENTC), in which the group has collaborative research projects that are exploring new electrophilic C-H activation catalysts and new direct routes to aromatic amines from benzene. Bill remains Associate Editor for the *The Journal of the American Chemical Society* for an eighth year, last year handling close to 500 manuscripts. He lectured in Sapporo, Eindhoven, Mexico, Nanjing, Quebec City, San Francisco, Wuhan, Shanghai, Toronto, Sevilla, Oviedo, and Taiwan, and was the closing speaker at the 2009 Gordon Conference on Organometallic Chemistry. One graduate student completed his degree, **BRETT SWARTZ (PH.D. '09)**, and is currently interviewing for industrial positions. Bill was also elected a Fellow of the American Association for the Advancement of Science in 2009.

The group's scientific accomplishments have centered upon our work in alkane C-H bond activation, in which we showed that a rhodium complex first binds to an alkane and then cleaves the C-H bond. Studies have shown that the metal will only break the C-H bonds in the terminal methyl groups. This selective feature was also surprisingly seen in the activation of 1-chloroalkanes and 1-cyanoalkanes. Investigations of competitions between various nitriles show a preference based on chain length, consistent with the notion that the metal binds

to the chain and then 'walks' down to the end before inserting. With chloroalkanes, the opposite is seen, i.e., all chain lengths compete 1:1. This led to the postulate that binding to the chlorine was rate determining, not the binding to the alkyl chain. Using kinetic techniques, it was determined that a rhodium-methyl bond is 3 kcal/mol stronger than a rhodium-cyanomethyl bond, yet C-H activation adducts of the latter are more stable because reductive elimination leads to the formation of a weaker C-H bond. This analysis is being applied to other substrates to come up with a global understanding of C-H activation thermodynamics.

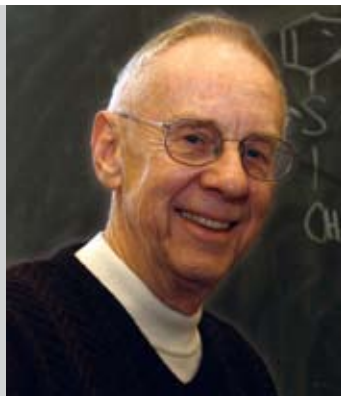
This work was described in August 2009 at the ACS National meeting in Washington, DC, where Bill received an ACS Arthur C. Cope Scholar Award. Our work in C-H activation is also continuing in a collaborative research effort in the Center for Enabling New Technologies through Catalysis (CENTC). This NSF-funded 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. 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 Prof. Juventino Garcia at the Universidad Nacional Autonomas de México.

Bill has also been invited back to China this fall to speak at the 3rd PKU-Lilly Symposium in Beijing. He will also speak in Durham at the 12th Dalton Discussions. He is also a member of the International Scientific Committee for the International Conference on Organometallic Chemistry, 2010 and 2012. The group is supported by continuing funding from the Department of Energy, the National Science Foundation, and the NSF Center Enabling New Technologies through Catalysis.

## Jack A. Kampmeier

Professor Emeritus of Chemistry

Ph.D. 1960, University of Illinois



### RESEARCH INTERESTS

Organic reaction mechanisms: free radical chemistry, organometallic reactions, and electron transfer reactions. Chemical education: The Peer-Led Team Learning Workshop.

### CONTACT

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**JACK KAMPMEIER** writes: The peer-led Workshop continued to break new ground at Rochester in the past year with the first adoption in the Humanities in Philosophy 101. In addition, colleagues in Biology and Biomedical Engineering worked to define ways to adapt the Workshop to laboratory teaching. This experimentation in lab teaching was initiated by Jim Farrar (in first-year chemistry), Joe Dinnocenzo (in Honors Organic Lab) and Carmela Garziona (in Geology 101) in 2008-9. The Fund for Workshop Education sponsored a return visit by Professors Richard Felder and Rebecca Brent to engage peer-leaders from across the campus in a Saturday morning session on the principles and practices of active learning. In a related pedagogical initiative, I continued to collaborate with Jerry

Mohrig from Carleton College to present a week-long workshop on "Teaching Guided Inquiry Organic Labs" at the University of Minnesota for 27 college teachers from across the country and the spectrum of higher education. The workshop was funded by NSF through the Center for Workshops in the Chemical Sciences at Georgia State.

Since 2005, I have been "Emeritus, but not retired." The academic year 2009-10 marked my 50th year with UR; it has been and continues to be exciting even though I no longer get paid. I celebrated the year with a birding safari in South Africa with my elder son Scott. Our target was 400 new species in 14 days; our final lists exceeded our expectations.

## Andrew S. Kende

Charles F. Houghton Professor Emeritus of Chemistry

Ph.D. 1957, Harvard University



### RESEARCH INTERESTS

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

### CONTACT

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Professor **ANDREW KENDE** and his wife, Frances, now reside full time in Scottsdale, AZ. They expect to be back in Rochester around August 25-27, 2010 as they return from attending the 240th American Chemical Society National Meeting in Boston, MA earlier that week. As a Director of Organic Reactions Inc., Prof. Kende plans to attend the August 23rd annual meeting of the O.R. Board of Directors in Boston. Prof. Kende again invites former UR graduate students, postdoctoral fellows and colleagues who plan to be in the Phoenix area to contact him via his UR email address well in advance of their travels to Arizona.







## 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 dynamics.

## CONTACT

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The **KRAUSS** group enjoyed another year of personnel accomplishment as several students and postdoctoral fellows moved on to more permanent positions. Congratulations to **LISA CARLSON (PH.D. '09)**, who successfully defended her thesis in August of 2009, and who, we are delighted to say, was the Outstanding Dissertation Award winner for the natural sciences! Lisa spent the past year teaching at Southern Connecticut State University and will be moving to a tenure track Assistant Professor of Chemistry position at Gannon University in the fall. Congratulations are also in order for **AMY ENSIGN (PH.D. '09)**, who graduated in August of 2009 and **SHUJING WANG (PH.D. '10)**, who defended her thesis in May of 2010. Amy is right here in Rochester teaching chemistry as a member of the faculty of Roberts Wesleyan College. Shujing is returning to her home town near Shanghai, China. Congratulations are also in order for Chris Evans, who was one of a handful of students selected to participate in the Egypt-U.S. Advanced Studies Institute conference in Cairo earlier this year. Last but certainly not least, Postdoctoral fellows **MARAT KHAFIZOV (POSTDOCTORAL FELLOW '10)** and **XIAOYONG WANG (POSTDOCTORAL FELLOW '10)** have started their independent careers: Marat is on the technical staff at Idaho National Laboratory while Xiaoyong is about to start a permanent position in Optics at Nanjing University in China.

Dr. Andrea Lee and Wesley Asher, both co-advised by Prof. Kara Bren, have been working very hard exploring various aspects of protein folding on the single particle level. They have had major breakthroughs in the last couple of months and are winning the year-long battle to acquire meaningful data. Julie Smyder painstakingly matched optical images and force microscope images to reveal that only a few percent of carbon nanotubes on a surface are actually emissive! This result was somewhat surprising and will affect the way carbon nanotubes are used in future applications. Jack Calcines is writing a paper (and finishing up a thesis!) on the role of secondary phosphines in the growth properties of semiconductor quantum rods.

Helen Wei partially succeeded in a very hard task: making "special" nonblinking quantum dots with potential for vastly im-

proved lasers and optical amplifiers, and she is working on a possible route to make the particles even better. Also, Jenneke Jalink succeeded in making vertically aligned carbon nanotube arrays, and is now putting those arrays into a thin polymer membrane for the production of hydrogen from solar energy. Fen Qiu and Brad Loesch are just getting started in their research. Fen is working on purifying highly fluorescent quantum dot-antibody conjugates for immunoassays, while Brad is exploring the fundamental triplet states of carbon nanotubes.

The group is delighted to have added four new students this year: Nicole Briglio, Kelly Sowers, Lenore Kubie and Cunming Liu. Nicole is working on using peptides to solubilize and sort carbon nanotubes while Kelly is growing semiconductor quantum rods and studying their fluorescence properties on the single molecule level. Lenore is another Krauss-Bren student who is interested in the photoinduced charge transport between heme containing proteins and carbon nanotubes. Lenore also won selection to participate in the University's Integrative Graduate Education and Research (IGERT) program on renewable energy, which will include a trip to Africa for several weeks to witness distributed solar energy firsthand! Cunming is our first materials science student who joined the group only one month ago. He is interested in both experimental and theoretical studies of quantum dots.

During the summer the group hosted Jessica Lucas from Simmons College, and she is going to lead our team in defense of the championship in the Krauss vs. Bren group mini golf tournament later this summer.

Finally, on a personal note, Todd was promoted to the rank of Professor of Chemistry this year. Todd thanks the many Chemistry faculty, Department staff, postdoctoral fellows, and students who have provided assistance and inspiration for these past 10 years at Rochester. Seems like he just got here.

## Robert W. Kreilick

Professor Emeritus of Chemistry

Ph.D. 1964, Washington University



### RESEARCH INTERESTS

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

### CONTACT

kreilick@chem.rochester.edu

**ROBERT KREILICK** is enjoying his third 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. Two years ago, new software was written for the ESR spectrometer and low temperature equipment was brought back into working order. We now have an ESR center which is being used by other chemistry faculty members.



*Rush Rhees Library from the University's baseball field*

## 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 to direct our NSF funded Research Experience for Undergraduates program. The 2010 REU program had a total of 25 participants, with 13 students from other schools together with 12 UR students. Five REU participants just completed their first year of college, which reflects our philosophy of starting students in research as soon as they are ready to do so. Last summer Tom attended an NSF REU site directors meeting in San Antonio to share 'best practices' for the summer program. As one of the longer-running REU programs, it was a plea-

sure to share our experiences. Tom also continues as Chair of the Chemistry Graduate Studies Committee, and 31 entering graduate students last September (2009) stimulated Tom to coordinate a revision of our faculty adviser selection process that ended up working well. Jing Qiao, who is working full-time for Momenta Pharmaceuticals in Boston, is writing her thesis on NMR structural studies of RNA hairpins; we hope to report successful completion of her thesis next year.

# David W. McCamant

Assistant Professor of Chemistry

Ph.D. 2004, University of California, Berkeley



## RESEARCH INTERESTS

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

## CONTACT

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The **MCCAMANT** group is doing well with science and life progressing well on all fronts. Our group was quite large for the 2009-2010 academic year, since we accepted two new graduate students into the group and had two undergraduates with us as well. In the fall, first year graduate students Randy Sabatini and Barbara Dunlop joined the group. Randy will be a joint student with Rich Eisenberg serving as co-advisor. He'll be pursuing studies of the ultrafast dynamics in molecular systems relevant to solar hydrogen production. Our group received funding in 2009 from the American Chemical Society's Petroleum Research Fund which supports a study to probe vibrational coupling in aromatic hydrocarbons and metallocenes using femtosecond stimulated Raman spectroscopy (FSRS). Barbara comes to us with a degree in Physics, and will join Kristina Wilson on the two-dimensional femtosecond stimulated Raman spectroscopy (2D-FSRS) project, which produced our first McCamant group publication in December!

Seniors **RANDY MEHLENBACHER (B.S. '10)** and **COLIN KINZ-THOMPSON (B.S. '10)** also did their senior research projects in the group. Randy continued his work on 2D-FSRS and produced a first-author publication in the *Journal of Chemical Physics* on the classical theory of this new technique. Randy

was honored with the Stoddard prize from the Department of Physics for the best senior thesis of the year and was a finalist for a prestigious Hertz graduate fellowship. Randy will start graduate school in the fall at the University of Wisconsin. Colin performed experimental and computational studies of reduced and oxidized nucleic acids and was responsible for putting together our new spectroelectrochemistry set up. Colin received an award for the best presentation at the undergraduate research expo in the spring, in which he presented his work with Prof. Conwell on simulations of hole dynamics in DNA helices. He will start graduate school at Columbia in the fall. Both of these talented undergraduates were a pleasure to work with and will be missed in the coming year.

Graduate student, Justin Rhinehart published his FSRS study of charge-transfer dynamics, but more importantly he and Jennifer Miller (of the Jones group) were married in July. The DNA photophysics work continues with the hard work of third-year graduate student, E. Ofotsu Djabeng, and postdocs Yong Du and J. Reddy Challa. Reddy joined us in November of 2009 and is pursuing studies of the ultrafast dynamics of DNA analogs such as 7-azaindole.

*The McCamant Group, Summer 2010*



## John S. Muentner

Professor Emeritus of Chemistry

Ph.D. 1965, Stanford University



### RESEARCH INTERESTS

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

### CONTACT

muentner@chem.rochester.edu

The academic year began well for **JOHN MUENTNER** as he enjoyed retirement but is still active in the Department, coming to seminars and attending Dave McCamant's research group meetings. Spectroscopy collaborations have continued with Carlo Callegari and with **MARK MARSHALL (B.S.'79)** and Helen Leung. Two papers have appeared this year, both in the Bob Field Festschrift. One describes the last work from my long collaboration with Tom Rizzo in Switzerland. The main author on this paper, Andrea Callegari, is the identical twin brother of Carlo Callegari, the principal

author of the helium nanodroplet paper. This work is from the Technical University in Graz, Austria and describes ESR measurements on single alkali metal atoms adsorbed on the surface of liquid helium nanodroplets. These experiments were done in the old Rochester molecular beam apparatus since it moved to Graz.

The year ended with great sadness when Annabel Muentner, John's wife of over 40 years, died after a long fight with breast cancer.

## 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; HIV infectivity and microbicide development.

### CONTACT

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The **NILSSON** group has made substantial progress in the last year. We are continuing studies of self-assembly phenomena with a focus on peptide and amino acid aggregation into amyloid-type structures. We have reported discoveries of amino acid derivatives that exploit aromatic effects to self-assemble in water into fibrillar hydrogel networks with high efficiency. We are currently exploring the mechanistic basis for these phenomena and are developing applications for these interesting materials. We have also developed a self-assembled peptide system that undergoes self-assembly and hydrogelation only in response to a reducing environment. This work was featured on the cover of *JACS* and was highlighted as an Editor's Choice paper in *Science*. In addition to these studies, we have also made excit-

ing progress in our study of the Alzheimer's disease A $\beta$  peptide. We have discovered methods to very efficiently block A $\beta$  self-assembly and prevent formation of neurotoxic congeners of this peptides. We have also made progress in understanding aspects of the biophysical driving forces for the self-assembly of this important peptide. We have also initiated a collaborative project with Professor Stephen Dewhurst (Department of Microbiology and Immunology, University of Rochester Medical Center) to study the effect of an amyloid peptide (SEVI) found in semen on HIV infectivity. We are also attempting to use model self-assembled peptide systems to mimic SEVI enhancement of HIV infection and to block these effects as possible microbicides. The Nilsson group received a CNIHR grant (Creative

and Novel Ideas in HIV Research, funded by the NIH) to perform this work.

The members of the Nilsson group have also made enormous progress in the last year. **TIMUR SENGUEN (PH.D. '10)** has completed his Ph.D. thesis research and is busy writing papers and thesis chapters in anticipation of his eminent graduation! Timur will be the first Ph.D. graduate from the Nilsson lab. He will move to Boston during the summer of 2010 to accept a postdoctoral research position at the Boston Biomedical Research Institute. Naomi Lee took a short leave of absence during the last year during which she enlisted in the Army National Guard and endured officer's training school. Naomi is back in lab working hard and hoping to complete her Ph.D. studies in the next year. Charlie Bowerman, Todd Doran, and Derek Ryan are all making tremendous strides in their research efforts. Todd and Derek will present their work at the National ACS meeting in Boston this summer and Charlie attended the Chemistry and Biology of Peptides Gordon Conference in March 2010. Charlie was selected to be a student organizer for the inaugural Chemistry and Biology of Peptides Gordon Research Symposium to be held in 2012 and he will also be on the organizing committee for the American Peptide Symposium in San Diego (summer 2011). John DiMaio and Ria Swanekamp completed the requirements for their M.S. degrees this year and advanced to candidacy for the Ph.D. degree. Both are making excellent

progress in their research. Wathsala Liyanage joined the Nilsson group this year. She comes to Rochester from Sri Lanka via New State University and she has been a welcome addition to the group. Our trusted postdoc, Beth Anderson, is keeping the group in line and has initiated collaborative efforts in the group to develop imaging agents for Alzheimer's disease.

**ALISSA KAMENS (B.S. '10)** performed her senior thesis research in the Nilsson lab this past year. She will continue to pursue Ph.D. studies in chemistry at Tufts University commencing Fall 2010. We wish her success in her future endeavors! Alex Federation and Sam Anderson have continued to conduct research in the Nilsson group. Sam has co-authored two papers in the group to date and Alex has conceived and initiated some exciting  $A\beta$  work in the lab that promises to be very high impact. Both are continuing work through the summer of 2010, Alex as a De Kiewiet fellow (University of Rochester, Biology Department). Nate Brown has also joined the Nilsson group this summer. Nate recently completed his freshman year and took the CHM 172Q/173Q courses taught by Brad. He was a phenomenal student and he is working on efforts to develop enantioselective catalysts for the synthesis of amino acid derivatives.

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

## Misha Ovchinnikov

Assistant Professor of Chemistry

Ph.D. 1995, University of Utah



### RESEARCH INTERESTS

Quantum dynamics of many-body systems; development of effective numerical methods based on semi-classical dynamics; applications to non-linear spectroscopy in the condensed phase.

### CONTACT

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Over the past seven years, the **OVCHINNIKOV** group has primarily focused on the development of new methods for solving many-body quantum dynamics problems. They have been developing effective numerical methods that can calculate quantum mechanical time evolution based on its semiclassical representation by classical trajectories. During the first half of Misha's seventh year of teaching and research in theoretical physical chemistry, research also continued on the development of a new method, the so-called Coherent State Path Integral (CSPI) semi-classical dynamics or "complex trajec-

tory" method. The Ovchinnikov group successfully applied this method to a number of test problems and began using it to solve exciting problems in quantum mechanics. At the end of 2009, Misha took leave of the Chemistry Department here at the University of Rochester to join Alcon Laboratories, Inc. in Irvine, California. Misha Ovchinnikov and his entire former research group are grateful for the support and friendship that everyone in the Chemistry Department extended to them during the past seven years.

# Lewis J. Rothberg

Professor of Chemistry

Ph.D. 1983, Harvard University



## RESEARCH INTERESTS

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

## CONTACT

rothberg@chem.rochester.edu

**LEWIS ROTHBERG's** group continues to work in diverse areas of science. Obtaining research funding has been difficult and Lewis has spent an inordinate amount of time raising grant funding this year. Those efforts are beginning to bear fruit and we are optimistic about the future. Along with Ching Tang and Shaw Chen in Chemical Engineering, we received a major grant from the Department of Energy for solid-state lighting using organic materials and another for enhancement of photovoltaics from NYSERDA with Philippe Fauchet. In addition, the University obtained a NSF grant for applications of photovoltaic technology in the Third World that will support Chris Favaro, a new student shared with Ching Tang. The other graduate students are progressing and the bodies of work by Millard Wyman and Steve Paquette are beginning to develop into Ph.D. theses. Kelly Sassin (Physics) is continuing her studies of organic light-emitting diodes as pertains to the solid-state lighting grant. She continues to work with our treasured colleagues, Dr. Al Marchetti and Dr. Ralph Young, whose expertise in organic electronics has immeasurably enriched the group's contributions. The excellent progress made by Chi-Sheng Chang (Materials Science) in synthesizing and applying new plasmonic particles to solar energy applications is the basis for the NYSERDA award. Xiao Wang (Biophysics and Structural Biology) is well along in making a new instrument under NSF funding that will enable us to attack novel biochemical binding problems using label-free interferometric detection and we are actively engaging several biochemically savvy collaborators to address high-impact problems in biomedicine.

We are blessed with a cadre of bright new students just beginning to ramp up their research. Ben Martin has finished his M.S. thesis on single chain polymer spectroscopy and the roadmap for his doctoral project is predicated on novel extensions of what he has done. Julianne Green and Chris Favaro are also beginning thesis projects in organic electronics. UR undergraduate Darcy Chen worked with us this year on polythiophene solvatochromism and her project will be continued by Jonathan Raybin who is already off to a great start. In addition, Emma

Spady from Swarthmore is spending the summer and working with Dr. Barbara Stwertka studying interactions of DNA with gold nanoparticles. Barbara's insight, energy and fearless approach to science have become one of the greatest joys at work for Lewis and are a huge benefit for the students in the group.

For the first time since 2003, Lewis taught graduate molecular spectroscopy (CHM 458) and struggled to keep up. The course format is unorthodox in that the lectures are problem solving, mostly from the literature, rather than theory and the students do about half of the lecturing. It seems to serve the purpose of helping students lose fear of the literature and transition to research but it is a lot of work for everyone. Some day, maybe a textbook will emerge from the course. Lewis once again taught the advanced spectroscopy lab (CHM 232) and once again was grateful for huge assists from Ray Teng, Ben Martin, **COLIN KINZ-THOMPSON (B.S. '10)** and **RANDY MEHLENBACHER (B.S. '10)**. Lewis presented work at a large number of meetings and institutional seminars.

Diffinity Genomics, a biotechnology company based on work started in the group, continues to rent R&D space in Hutchison and has progressed to the point where they opened a manufacturing facility in Henrietta. The company began selling a first product, pipette-based polymerase chain reaction cleanup kits, receiving their first purchase orders in May. During the year, Diffinity hired a second Ph.D. Chemist, William Begley, and he has made big contributions to their success. It is gratifying to see the impact of the science and we hope that the presence of the excellent scientists and exciting work contributes to the education of the students.

Shelby, Lewis, Charles (7), and Vivian (6) are thriving. Shelby is super-busy with high profile projects at Kodak while making home life rich and delightful. Charles is enjoying sports and early reading while Vivian loves art and "can't wait" to get homework from school too.

## William H. Saunders

Professor Emeritus of Chemistry

Ph.D. 1952, Northwestern University



### RESEARCH INTERESTS

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

### CONTACT

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**BILL SAUNDERS** writes: In June I took a trip to France – 3 days in Paris followed by a bike trip in the Loire Valley region. We visited all of the major chateaux and had good food everywhere. I was the only person in the group of bikers who had had any formal instruction in the French language, so I acquired a wholly undeserved reputation for fluency. The rest of the summer included two trips to the Stratford, Ontario Shakespeare Festival, one of them with my daughter and two granddaughters. The last event of the summer was a visit from an old English friend, Anthony Roe, in late August and early September. Anthony was a postdoc at Rochester in the

late 1950's, when I was a very junior faculty member. In November I attended the Physical Organic Minisymposium at the University of Buffalo. The whole family spent Christmas at Claude's home in Oak Park, IL. In February I attended the Gordon Isotopes Conference, which this time was moved from its longtime location in Ventura, CA to Galveston, TX. As a city, Galveston suffers by comparison to Ventura, but the science at the meeting was very interesting. I finally got around to writing up the valence bond calculations on elimination reactions. The paper was accepted by the *Journal of Organic Chemistry* and appeared in May.

## 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. Chemi- and physisorption of tritium in metals.

### CONTACT

schroeder@chem.rochester.edu

**UDO SCHRÖDER**'s group continued research in radio-chemistry, heavy-ion reaction dynamics, as well as in technical R&D. Experimental and theoretical results on cluster emission in heavy-ion induced reactions have been presented by several group members at national and international conferences. The emphasis in this work has been on the apparent similarities between cluster emission from hot, expanded nuclei and their production in a hypothetical liquid-gas phase transition for finite nuclei. The most recent application of the model has been in explaining regularities ("isoscaling") in the isotopic distributions of fragments emitted in statistical disintegration of nuclei at the limits of stability. This area remains an important research focus by the group. Last winter, two chemistry grad students participated in a new experiment at LNS Catania, where nucleon transfer is studied for a very neutron rich and a neutron poor reac-

tion system. Group members presented talks at ACS and APS meetings. Udo gave an invited lecture at the San Francisco Seaborg Symposium and the Symposium on Nuclear Symmetry Energy in Noto, Italy, in addition to research seminars in UR Departments.

Last semester, for the first time, the Advanced Nuclear Science Education Laboratory (ANSEL) was taken by an inaugural class of undergraduate and graduate students from Chemistry, Physics and Engineering. The lab has been funded by a grant from the NRC and been strongly supported by the Chairs of Chemistry and Physics Departments, as well as by the Medical Center and the Laboratory for Laser Energetics. In its first run, the ANSEL was considered a great success by all involved, especially by the students.

# 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's** graduate student **CEN GAO (PH.D. '09)** successfully completed his Ph.D. in Fall 2009, and has started a postdoc at UNC Chapel Hill in their new Center for Integrative Chemical Biology and Drug Discovery. A good chunk of Cen's thesis work, on accounting for the free energy cost of ligand conformational change in binding affinity calculations, was recently published in *Biophysical Journal*. Graduate student Min-Sun Park has been working extremely hard on (at least) three projects. One of these is examining the structure and dynamics of the binding interface of the  $\beta\gamma$  subunit of the G protein, when complexed with various partners (phosducin, the G protein  $\alpha$  subunit, and a high-affinity peptidic ligand). Min-Sun contributed some results to a paper published in PNAS and is also preparing a manuscript for submission to *Proteins: Structure, Function, Bioinformatics*. Min-Sun has also been working on attacking another tough problem in binding affinity calculations – dealing with variable protonation states in the ligand and receptor binding pocket, and proton uptake/release upon binding. Finally, in collaboration with Ha Youn Lee and Sung Yong Park in the UR Department of Biostatistics and Computational Biology, Min-Sun has been working on modeling complexes of oligopeptide epitopes to the major histocompatibility complex, with the goal being computer-aided discovery of new peptidic vaccines. Undergraduate Maruf Sarwar, unfazed by a whole semester of Harry in P-Chem, is working with the group this summer as an REU student. He will be collaborating with Prof. Tina Iverson's group at Vanderbilt University (coincidentally located in his hometown!) on modeling complexes of fumarate reductase, an enzyme that is part of the anaerobic respiratory chain in prokaryotes, to various dicarboxylate ligands, to try to understand why some are substrates and some inhibitors.

Harry and Alison were blessed with the arrival of Connor Gordon Stern in Fall 2009. He is a good-natured and easy baby. As of press time, the little guy has somehow managed to survive eight months with Eva and Danny, so we think he will be able to handle anything life throws his way. Eva will be starting kindergarten in Fall 2010 and resembles a small teenager (likes to sleep late, has figured out that her dad knows virtually nothing

about the world, and eats a lot of mac & cheese late at night). Danny will be three in October and is more like some kind of natural disaster involving high winds and flooding. When not experimenting with the toilet or waking his mom up from a nap with a friendly body slam, he enjoys playing with his favorite toys in the garage such as the pruning shears, hedge trimmer, and snow blower.

*Interfaith Chapel from the Genesee River level*





# Douglas H. Turner

Professor of Chemistry

Ph.D. 1972, Columbia University



## RESEARCH INTERESTS

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

## CONTACT

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This year's science reflected the interdisciplinary and collaborative approach of the **TURNER** group's studies of RNA. Biao Liu developed and published a fluorescence competition assay for measuring the thermodynamics of formation of RNA pseudoknots, an important motif with almost no experimental rules for predicting the sequence dependence of stability. Biao collaborated with **DAVE MATHEWS (B.S. '94, PH.D. '02, M.D. '03)** to also publish an invited review article about pseudoknots. In collaboration with Scott Kennedy and Ryszard Kierzek, Nic Hammond published NMR structures of five RNA duplexes with AG internal loops. They discovered a completely new 3D motif for the sequence, 5'GAGU/3'UGAG. It was expected to have AG pairs flanked by GU pairs, but instead the major conformation has two bulged out U's and two GG pairs that flank an AA pair. All the G's are syn and it was only possible to determine the structure because Ryszard synthesized sequences with 8-bromo or 8-methyl G. It would be great to know why RNA forms various 3D motifs. In a step toward such understanding, **ILYAS YILDIRIM (PH.D. '08)** collaborated with Harry Stern on quantum calculations to provide new parameters for molecular dynamics simulations of RNA. To test predictions of the simulations, Ilyas worked with Jason Tubbs and Scott Kennedy to use NMR to determine structural features of nucleosides and of a single stranded oligonucleotide. The new parameters reproduce the NMR determined features much better than parameters that have been widely used. Ilyas, Doug, and Dave Mathews also collaborated on a project in Jiri Sponer's lab to test the stability of three known 3D structures of a particular internal loop found in ribosomes. To Doug's relief, the NMR structure published by **NEEL SHANKAR (PH.D. '07)** in 2006 is stable in molecular dynamics simulations whereas the structures in ribosomes are not. Evidently, the structures in ribosomes reflect interactions with the environment, rather than intrinsic properties of the RNA. The papers with Ilyas were both published in the *Journal of Chemical Theory and Computation*, which represents a new direction of the Turner group toward collaborations with computational chemists. In August, Ilyas started a postdoc with George Schatz at Northwestern University.

Doug and Ilyas also helped the Kierzek group with a study that showed stability and specificity of RNA recognition by probes is enhanced by substituting LNA-2-thiouridine for 2'-O-methyluridine. For many years, the Turner group has measured the sequence dependence of RNA thermodynamics by optical melting and thus Doug and **SUSAN SCHROEDER (B.S. '95, PH.D. '02)** published an invited review on how to do it. Doug and Dave Mathews published a paper announcing Dave's new website with a compendium of the thermodynamic results so that they can be easily accessed by groups writing computer programs for predicting properties and functions of RNA. Even without such a website, Dave's 1999 paper in the *Journal of Molecular Biology* recently passed 2000 citations.

Former members of the group continue to prosper. This year, **MATT DISNEY (PH.D. '02)**, Dave Mathews, and **BRENT ZNOSKO (PH.D. '04)** received tenure, respectively, at SUNY Buffalo, UR, and St. Louis University. Following hockey terminology, Doug considers this a tenure "hat trick" for the group. Matt actually received two tenures and will move to the Scripps Institute in Florida this summer. So, he will move from SUNY Buffalo to sunny Florida. Does that count as a "hat plus glove trick" for the group? Matt also received a Dreyfus Teacher-Scholar Award. **GANG CHEN (PH.D. '05)** accepted a faculty position starting this summer at Nanyang Technological University in Singapore. Jim Hart (**PH.D. '10, M.D. '10**) received both his Ph.D. and M.D. and took a full time position at Abbott Labs in Dallas. Two new students, David Condon (Penn State) and Tian Jiang (Fudan University) joined the group to follow in the footsteps of the previous graduates. "A rising tide raises all ships." Two more senior students, Walter Moss and Indee Dela, followed in the footsteps of Matt Disney and **JESICA CHILDS (PH.D. '03)** by getting married.

Doug gave talks at SUNY Buffalo and in Berkeley at the 80th birthday celebration of his postdoctoral advisor, Nacho Tinoco. The latter event was also attended by former students **JOHN JAEGER (PH.D. '89)**, **MING WU (PH.D. '96)**, **SHENGHUA DUAN (PH.D. '06)**, and Gang Chen, along with former post-

continued on next page 



*Hutchison Hall from Bausch and Lomb Riverside Park*

doc **SUE FREIER**, which made it extra special for Doug. It was also special to have Ela and Ryszard Kierzek visit last summer to start a new collaborative project. This Spring, current student, Sal Priore, spent several weeks at the Kierzek lab in Poland to advance the collaboration.

The interdisciplinary nature of the lab's research was noticed by somebody at NSF, so Doug served on a panel reviewing proposals for Integrative Graduate Education and Research Training. In another attempt to facilitate interdisciplinary research, Doug and the Biological Chemistry Cluster expanded the Biological Chemistry Retreat to the Chemistry-Biology-Biophysics Interface Retreat (see separate article). Doug has been Director of the BC Cluster since its inception 6 years ago, and is thankful that Kara Bren will take over the leadership. The Provost supported the Cluster for the last five years so that the Chemistry Department only had to provide \$90, which funded the first Retreat. Doug's major regret is that he did not improve the quality of cookies at biologically relevant seminars.

Doug taught General Chemistry again this Spring. The required creative project for students was to write a poem about chemistry that used some material covered during the semester. Doug enjoyed the weekend reading the hundred poems, which included sonnets, free verse, limericks, haiku, and rap. The only disappointment was that Doug could not convince the rap writers to perform.

## 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. A particular focus of the past year has been the new reductive methods for the coupling of two electrophiles. Daniel Everson (2nd year Ph.D. student) and Ruja Shrestha (3rd year Ph.D. student) recently finished work on a general, nickel-catalyzed method for the coupling of aryl halides with alkyl halides. This new method formed the desired alkylated arene products in high yield under mild conditions – the reaction even tolerates air and water. Part of the reason the reactions are so tolerant is that the only apparent organometallic intermediates are catalyst-derived or-

ganonickel species, which are stable relative to Grignard or organozinc reagents. Another intriguing finding is that, in this case, a combination of two ligands is better than either ligand alone. These features, and the ability to utilize simple organic halides in place of pre-formed organometallic reagents, were highlighted in the secondary literature (C&E News, Synfacts). Daniel Everson will continue to work on this project, especially on expanding substrate scope to less reactive alkyl chlorides and tosylates and to heterocyclic substrates. Ruja has moved onto the reductive coupling of organic halides with other electrophiles, and we will report back on that work next year. Michael Prinsell (2nd year Ph.D. student) and Dan-

iel Everson also recently developed the first general method for the dimerization of alkyl halides less reactive than alkyl iodides, and a nickel catalyst also mediates this new reaction. As in our earlier work, the reactions trade pre-formed organometallic reagents for alkyl halides, allowing for true mix & stir simplicity. In this case, Mike found that the reaction is also easily scalable, with reactions at 2 mmol and 40 mmol scale resulting in the same high yield (96%) and similar reaction times. Another interesting finding in this work was that less reactive or unreactive substrates (alkyl chlorides, mesylates, and even trifluoroacetate esters) could be made to dimerize by the addition of catalytic amounts of sodium iodide (the iodide source in iodized table salt). These results have been recently published and will be the foundation for Mike's ongoing work in the formation of  $Csp^3-Csp^3$  bonds. Finally, Alex Wotal (first year Ph.D. student) has finished with his coursework and will continue his studies on the development of new reductive coupling methods that he began last summer.

Very recently, Marina Naodovic joined the group as our first postdoctoral researcher and has been working to push our chemistry in new directions that include C-X as well as C-C bond formation. She was joined this summer by our first undergraduates: Jessica Christiano, Brittany Jones, and Rachel

Kelemen. We also hosted two new graduate students on rotations this summer, Lukiana Anka-Lufford and Annada Rajbhandary, which brought our group size up to ten from only four last summer!

Outside of research, group members passed some significant milestones in the past year. Mike and Daniel passed their cumulative exams and are preparing for their oral exams. Ruja passed her oral exam and is now focused on thesis research full time. Daniel was awarded a National Science Foundation Graduate Research Fellowship, a great honor both for him and our department. Finally, Daniel and Mike both won the W. D. Walters teaching award. On a personal note, Daniel Everson married his long-time sweetheart Kelsey, and Daniel Weix was blessed with the birth of his and Stella's third child, Amalia, in July of 2009. We all continue to discover what Rochester has to offer during our free time. Recent discoveries are Roc-City Rollerderby, Chuck-E-Cheese, the Adirondacks, Letchworth state park, and Tony Pepperoni pizza. Daniel, Stella, Elliott, Madeleine, and Amalia continue to enjoy living in Rochester, especially eating fish fry from Hungry's by the canal, catching frogs in our back yard, and visiting Seabreeze.

*The Weix Group, Summer 2010*



*Includes publications accepted or submitted between July 2009 and June 2010.*

## ROBERT K. BOECKMAN, JR.

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## KARA L. BREN

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## ESTHER M. CONWELL

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## JOSEPH P. DINNOCENZO

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## RICHARD EISENBERG

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## SAMIR FARID

Bimolecular Electron Transfers that Follow a Boltzmann Dependence on Free Energy. S. Farid, J. P. Dinnocenzo, P. B. Merkel, R. H. Young, D. Shukla, *J. Am. Chem. Soc.*, submitted.

## JAMES M. FARRAR

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## ALISON J. FRONTIER

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## PATRICK L. HOLLAND

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## WILLIAM D. JONES

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*continued on next page* 

## JACK A. KAMPMEIER

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## LEWIS J. ROTHBERG

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## WILLIAM H. SAUNDERS

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## HARRY STERN

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## CHING W. TANG

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## DOUGLAS H. TURNER

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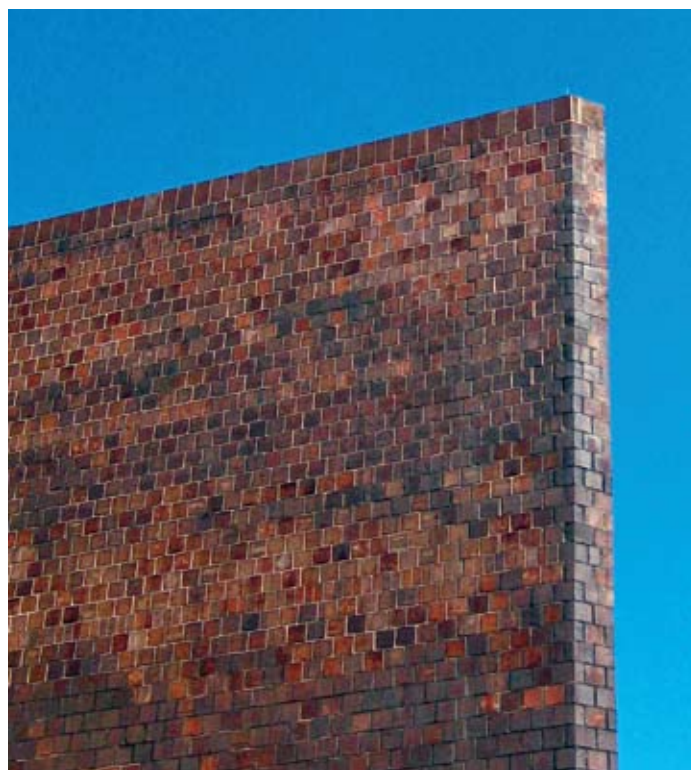
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## DANIEL J. WEIX

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Wilson Commons



## Bachelors and Masters Degrees Awarded in Chemistry

### 2010 BACHELOR OF SCIENCE

Daniel Cuneo<sup>1†</sup>  
David Farkas<sup>1</sup>  
Matthew Golder<sup>2</sup>  
Karen Horovitz  
Alissa Kamens<sup>3</sup>  
Colin Kinz-Thompson<sup>3†</sup>  
Brian Matthew Lindley<sup>3†</sup>  
Randy Mehlenbacher<sup>3†</sup>  
Alexander Sokolsky<sup>3†</sup>  
Jacqueline Zaengle<sup>2†\*\*</sup>

### 2010 MASTER OF SCIENCE

Stanislav Bellaousov  
Sarina Bellows  
Joshua Brooks  
John DiMaio  
Ofotsu Djabeng  
Daniel Everson  
Eric Glowacki  
Eric Henry  
Jenneke Jalink  
Erin Knappen  
Brendon Lyons  
Fen Qiu  
Jessica Smith  
William Spencer  
Ria Swanekamp  
David Turner  
Xiaoju Zhang

### 2010 BACHELOR OF ARTS

David Chadsey<sup>2</sup>  
Jonathan Chester\*  
Michael Collins<sup>1</sup>  
Alyssa Cowell<sup>1</sup>  
John R. Dakin  
John Foote<sup>3†</sup>  
Rakushumimarika  
Harada  
Nora Homs<sup>2</sup>  
Ethan Isaac Kaplan  
Calvin Lee  
Jason Lee<sup>1</sup>  
Michael Vito Mungillo<sup>2</sup>  
John Charles Oakford<sup>1\*</sup>  
Adi Robinson  
Devin Ruiz  
Julie M. Tabroff<sup>3†</sup>  
Kishan Tarpara

### DISTINCTIONS

<sup>1</sup>Distinction

<sup>2</sup>High Distinction

<sup>3</sup>Highest Distinction

<sup>†</sup>Phi Beta Kappa

\*Take 5 Scholar (finishing)

\*\*Take 5 Scholar (beginning)

<sup>†</sup>Kauffman Entrepreneurial Fifth Year (KEY) Student

*Class of 2010 Bachelor's Degree Recipients*





# Doctoral Degrees Awarded in Chemistry

## Abdallah Bitar

*Progress Toward the Total Synthesis of Roseophilin*  
Alison J. Frontier  
M.D./Ph.D., University of Rochester

## Lisa Carlson

*Photophysics of Individual Single-Walled Carbon Nanotubes*  
Todd D. Krauss  
Assistant Professor, Gannon University

## Keying Ding

*Synthesis and Reactivity of Low-Coordinate Cobalt Dinitrogen, Hydride and Fluoride Complexes*  
Patrick L. Holland  
Postdoctoral Fellow, University of Minnesota

## Amy Ensign

*Studies of Horse Heart Cytochrome c Folding*  
Kara L. Bren & Todd D. Krauss  
Assistant Professor, Roberts Wesleyan, Rochester, NY

## Cen Gao

*Computational Studies on Membrane Protein Structures and Protein-Ligand Binding Affinities*  
Harry A. Stern  
Postdoctoral Fellow, University of North Carolina at Chapel Hill

## Nathan Genung

*I) Studies Towards the Total Synthesis of +/- Lycoramine II) Development of the Retro-Aza-Claisen Rearrangement to Synthesize Medium Sized N-Substituted Heterocycles III) Studies Towards the Total Synthesis of (-)-Nakadomarin A*  
Robert K. Boeckman, Jr.  
Postdoctoral Fellow, University of California, Irvine

## James Hart

*NMR-Assisted Prediction of RNA Secondary Structure*  
Douglas H. Turner  
Systems Engineer, Abbott Labs in Dallas, TX

## Chao Jiang

*I) Stereoselective Synthesis of Pyrrolidine Derivatives via Reduction of Substituted Pyrroles II) Progress Towards the Total Synthesis of Tetrapetalone A*  
Alison J. Frontier  
Postdoctoral Fellow, University of Illinois, Champaign-Urbana, IL

## John Miller

*I) Direct Enantioselective Organocatalytic Hydroxymethylation of Aldehydes II) Synthesis of a Novel Bicyclic Amine Organocatalyst*  
Robert K. Boeckman, Jr.  
Postdoctoral Fellow, Stanford University

## Yan Miller

*I) Asymmetric Diels-Alder Reaction of Cyclic Isoimidium Salts II) Total Synthesis of a Camphor Derived Dimer III) Asymmetric Cyclopropanation*  
Robert K. Boeckman, Jr.  
Postdoctoral Fellow, Stanford University

## Sara Rocks

*Modeling Ring Cleaving Dioxygenases: Complexes of Iron(II) with Tridentate Ligands and their Reactivity with Catecholates and Phenolates*  
Patrick L. Holland  
Postdoctoral Fellow, Princeton University

## Brett Swartz

*The Investigation of C-CN Cleavage of Allyl- and Aryl-nitriles by [(dippe)NiH]<sub>2</sub> and [(dippe)PtH]<sub>2</sub>*  
William D. Jones

## Shujing Wang

*Ultrafast Spectroscopy of Single-Chirality Single Walled Carbon Nanotubes*  
Todd D. Krauss

University of Rochester Degree Covers



# Student Awards

## DEPARTMENT AWARDS

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

Randy Mehlenbacher

### **John McCreary Memorial Prize**

Colin Kinz-Thompson

### **ACS Rochester Section Award**

Matthew Golder

### **ACS Inorganic Chemistry Award**

Brian Lindley

### **Merck Index Award**

Alissa Kamens

### **Chemistry Department Award**

John Foote

Alexander Sokolsky

Julie Tabroff

## ENDOWED DEPARTMENT FELLOWSHIPS

### **Robert and Marian Flaherty DeRight Fellowship**

Karen Chiang

Meagan Evans

Gerald Manbeck

### **Elon Huntington Hooker Fellowship**

Thomas Dugan

Chris Evans

Ting Li

### **Arnold Weissberger Fellowship**

Walter Moss

Michael Quinlan

### **Samuel Allen and Ellen Frances Lattimore Fellowship**

Jennifer Ciesielski

Meghan Clark

Erin Knappen

Ruja Shrestha

Tulaza Vaidya

### **Agnes M. & George Messersmith Fellowship**

Sarah Bowman

## COLLEGE AWARDS

### **Ayman-Amin Salem Award**

Matthew Golder

### **Wendy Jill Fread Prize**

Randy Mehlenbacher

### **Janet Howell Clark Prize**

Julie Tabroff

### **Catherine Block Memorial Fund Prize**

Caitlyn Rose Kennedy

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

Meghan Clark

## TEACHING AWARDS

### **W. D. Walters Teaching Award**

Sarina Bellows

Daniel Everson

Chris Favaro

John Frost

Erin Knappen

Michael Prinsell

William Spencer

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

David Chadsey

Brian Lindley

Julie Tabroff

## PHI BETA KAPPA

Daniel Cuneo, John Foote, Colin Kinz-Thompson, Brian Matthew Lindley, Randy Mehlenbacher, Alexander Sokolsky, Julie M. Tabroff, Jacqueline Zaengle

# Fellows '09-'10

## Elizabeth Anderson

State University of New York at Stony Brook

## Jagannadha (Reddy) Challa

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

## Marco Cristani

Faculty of Chemistry, U.N.A.M., Mexico

## Yong Du

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

## Ajdin Kavara

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

## Marat Khafizov

University of Rochester-Physics; Middle East Tech University, Ankara, Turkey

## Sabuj Kundu

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

## David Leboeuf

Université Pierre et Marie Curie (UPMC)

## Andrea Lee

University of Wisconsin-Madison, Madison, WI

## Matthew Liptak

University of Wisconsin-Madison, Madison, WI

## Genggeng Luo

Xiamen University, Xiamen, P.R. China

## Satyanarayana Maragani

University of Pune, India; Pondicherry University, Pondicherry, India

## Theresa McCormick

Queen's University, Kingston, Ontario, Canada

## William McNamara

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

## Marina Naodovic

University of Chicago; University of Novi Sad, Serbia

## Alexey Novikov

Technische Universität Chemnitz, Chemnitz, Germany

## Hardey Singh

Panjab University, Chandigarh, India

## Taro Tanabe

Institute for Chemical Research, Kyoto University, Kyoto, Japan

## Francesca Vitali

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

## Xiaoyong Wang

University of Arkansas, Fayetteville, AR

## Ilyas Yildirim

University of Rochester- Physics; KOC University, Istanbul, Turkey

## Jing Zhang

Nanjing University, P.R. China

## Kaidong Zhang

University of Manitoba, Canada; Lanzhou University, China

*Greek Columns on the Fraternity Quad*



# Seminars & Colloquia

## JULY 2009

Professor Chaim N. Sukenik (Bar Ilan University, Israel) “*Chemical Control of Interfacial Composition and Structure*,” July 8, 2009.

Professor Michael S. Strano (Massachusetts Institute of Technology) “*Single Molecule Biodetection and Multi-Modality in Single Walled Carbon Nanotube Optical Sensors*,” July 10, 2009.

## AUGUST 2009

Lisa Joanne Carlson (University of Rochester) “*Photophysics of Individual Single-Walled Carbon Nanotubes*,” August 6, 2009.

Amy A. Ensign (University of Rochester) “*Studies of Horse Heart Cytochrome c Folding*,” August 10, 2009.

Chao Jiang (University of Rochester) “*I. Stereoselective Synthesis of Pyrrolidine Derivatives via Reduction of Substituted Pyrroles; II. Progress Towards the Total Synthesis of Tetrapetalone A*,” August 10, 2009.

Professor Oleg Prezhdo (University of Washington) “*Excitation Dynamics in Nanoscale Materials for Solar Energy Harvesting*,” August 25, 2009.

## SEPTEMBER 2009

Professor Lance Seefeldt (Utah State University) “*Insights into the Nitrogenase Mechanism*” September 9, 2009.

Professor Mark Distefano (University of Minnesota) “*Bioorganic Chemistry of Protein Prenylation*,” September 11, 2009.

Professor Philippe Hiberty (Université of Paris- Sud XI) “*New Concepts in Chemical Bonding: Charge Shift Bonding and its Manifestations in Chemistry*,” September 16, 2009.

Professor Matthew Disney (University of Buffalo) “*Progress Towards a Chemical Code for Small Molecule Targeting of RNA*,” September 18, 2009.

Sara S. Rocks (University of Rochester) “*Modeling Ring Cleaving Dioxygenases: Complexes of Iron(II) with Tridentate Ligands and Their Reactivity with Catecholates and Phenolates*,” September 18, 2009.

## VICTOR J. CHAMBERS MEMORIAL LECTURE

Professor Barry M. Trost (Stanford University)

I. “*On the Design of Chiral Space for Asymmetric Induction in a Catalytic Synthetic Reaction*,” September 21, 2009.

II. “*Self Assembly of Dinuclear Main Group Catalysts for Asymmetric Synthesis*,” September 22, 2009.

III. “*The Alkyne Strategy for the Synthesis of Bioactive Targets*,” September 23, 2009.

Professor Justine P. Roth (Johns Hopkins University) “*Strategies in Enzymatic Oxidation Catalysis*,” September 28, 2009.

Cen Gao (University of Rochester) “*Computational Studies on Membrane Protein Structures and Protein-Ligand Binding Affinities*,” September 29, 2009.

Karen Chiang (University of Rochester) “*An Introduction to Supercritical CO<sub>2</sub> (sc CO<sub>2</sub>) and Examples of Increased Selectivity in Reactions Due to the Properties of sc CO<sub>2</sub>*” September 29, 2009.

Professor Cathleen Crudden (Queens University, Ontario) “*Catalysis and Chirality with Molecules and Materials: Novel Catalytic Processes and Materials*,” September 30, 2009.

## OCTOBER 2009

## HARRISON HOWE LECTURE

Professor Carolyn R. Bertozzi (University of California, Berkeley)

I. “*Imaging the Glycome with Bioorthogonal Chemistry*,” October 1, 2009.

II. “*Research at the Intersection of Nanoscience and Biology- Highlights from the Molecular Foundry*,” October 1, 2009.

Professor Daniel Seidel (Rutgers University) “*Enantioselective Organocatalysis and the Study of Redox Neutral Reaction Cascades*,” October 2, 2009.

## HUTCHISON MEMORIAL LECTURE

Professor Kenneth N. Raymond (University of California, Berkeley)

I. "Human and Bacteria: The Arms Race for Iron," October 12, 2009.

II. "Supramolecular Metal Complexes as Nanozymes," October 13, 2009.

III. "Imaging with Lanthanides," October 14, 2009.

Professor Steven Corcelli (University of Notre Dame) "Computational Studies of DNA Hydration Dynamics," October 19, 2009.

Dr. Garry Rumbles (National Renewable Energy Laboratory) "The Dissociation of Excitons in Conjugated Polymers: Advancing Organic Solar Cells through Basic Research," October 21, 2009.

Professor Arthur Suits (Wayne State University) "What Do Roaming Radicals, Astrochemistry, Proteomics and Atomic Orbital Polarization Have in Common?," October 26, 2009.

Ryan Cowley (University of Rochester) "Caught in the Middle: Formation and Reactivity of Magnesium(I) Compounds," October 27, 2009.

Professor David Collum (Cornell University) "Structure-Reactivity Relationships in Organolithium Chemistry: Working at the Academic-Industrial Interface," October 28, 2009.

Professor Matthias Brewer (University of Vermont) "Ring Fragmentations and Intramolecular Cycloadditions: Efficient Approaches to Nitrogen Heterocycles," October 30, 2009.

## NOVEMBER 2009

Professor Dean Wilcox (Dartmouth College) "Thermodynamics of Metal-Protein Interactions: Essential Metal Transport and Toxic Metal Sequestration," November 2, 2009.

Dr. Sergei Tretiak (Los Alamos National Laboratory, Theoretical Division) "Modeling of Photoinduced Dynamics at the Nanoscale," November 4, 2009.

Professor Bradley Holliday (University of Texas at Austin) "Functional Conducting Metallopolymer Materials," November 9, 2009.

Professor Jason Gestwicki (University of Michigan) "Allosteric Regulation of Heat Shock Protein 70 by Small Molecules," November 13, 2009.

Professor Mark Tuckerman (New York University) "Topological Charge Defects in Hydrogen-Bonded Systems Probed by Ab Initio Molecular Dynamics: Bulk and Interfacial Properties," November 16, 2009.

Professor Samuel Gellman (University of Wisconsin, Madison) "Structure and Function in Peptidic Foldamers," November 18, 2009.

Professor Jeffrey D. Hartgerink (Rice University) "Self-Assembling Collagen Triple Helices and Beta-Sheet Nanofibers," November 20, 2009.

## DECEMBER 2009

Brett David Swartz (University of Rochester) "The Investigation of C-CN Cleavage of Allyl- and Aryl-nitriles by [(dippe)NiH]<sub>2</sub> and [(dippe)PtH]<sub>2</sub>," December 7, 2009.

Stephen Paquette (University of Rochester) "Suppression of Photobleaching in Tris-8-(hydroxyquinoline) Aluminum Through Plasmon Enhanced Spontaneous Emission," December 11, 2009.

Nathan Edward Genung (University of Rochester) "I. Studies Towards the Total Synthesis of +/- Lycoramine; II. Development of the Retro-Aza-Claisen Rearrangement to Synthesize Medium Sized N-Substituted Heterocycles; III. Studies Towards the Total Synthesis of (-)-Nakadomarin A," December 11, 2009.

## JANUARY 2010

Professor Torben Lund (Roskilde University, Denmark) "Degradation Chemistry of the Dye Sensitized Solar Cell (DSC) Ruthenium Dyes," January 14, 2010.

Thomas Dugan (University of Rochester) "Aryl Carbon-Fluorine Bond Formation Promoted by Transition Metal Complexes," January 15, 2010.

Millard Wyman (University of Rochester) "Factors Affecting Charge Utilization in Conjugated Polymers," January 20, 2010.

Gerald Manbeck (University of Rochester) *"Two-Dimensional Cruciform Functional Materials: Applications from Single Molecule Switches to Fluorescence Sensing,"* January 22, 2010.

Mehmet Can (University of Rochester) *"Genetically Engineered Oxygen-Carrying Blood Substitute: Variants of Human Serum Albumin,"* January 25, 2010.

Matthew Grochowski (University of Rochester) *"Reactivity of Saturated Hydrocarbons in Super Acids,"* January 26, 2010.

Jennifer Miller (University of Rochester) *"Catalysis Using Palladium(IV) Intermediates,"* January 29, 2010.

## FEBRUARY 2010

Jennifer Ciesielski (University of Rochester) *"Reactions of Siliranes with Carbonyl Compounds,"* February 5, 2010.

Justin M. Rhinehart (University of Rochester) *"Intramolecular Charge Transfer in 4-(Dimethylamino) benzonitrile (DMABN),"* February 8, 2010.

Professor Christopher Bauer (University of New Hampshire) *"Curriculum Assessment Research in the Teaching and Learning of Chemistry,"* February 15, 2010.

Dr. Theresa McCormick & Derek Ryan (University of Rochester) *"I. Artificial Photosynthesis: Photo-Splitting of Water Using a Molecular Cobalt Catalyst; II. Probing the Role of Aromatic Interactions in Molecular Self-Assembly,"* February 17, 2010.

Charles J. Bowerman (University of Rochester) *"Block Copolymers via ROMP for Multivalent Ligand Display,"* February 19, 2010.

Professor Paul Chirik (Cornell University) *"Base Metal Catalysis: The Interplay of Electronic Structure and Reactivity,"* February 22, 2010.

Professor Kevin Burgess (Texas A & M University) *"Chiral Crabtree Catalyst Analogs for Syntheses of Valuable Chirons,"* February 24, 2010.

Todd Doran (University of Rochester) *"The Chemical Synthesis of Glycoproteins,"* February 26, 2010.

## MARCH 2010

Professor Alexander Shestopalov (University of Rochester) *"Alternative Printing and Fabrication Techniques for Chemical Nano-Patterns and Functionalized Janus Particles,"* March 1, 2010.

Yan Miller (University of Rochester) *"I. Asymmetric Diels-Alder Reaction of Cyclic Isoimidium Salts; II. Total Synthesis of a Camphor Derived Dimer; III. Asymmetric Cyclopropanation,"* March 2, 2010.

Professor John Papanikolas (University of North Carolina at Chapel Hill) *"Ultrafast Dynamics in Complex Systems,"* March 3, 2010.

Brian Ohman (University of Rochester) *"A New Development in Simmons-Smith Cyclopropanation,"* March 5, 2010.

John Miller (University of Rochester) *"I. Direct Enantioselective Organocatalytic Hydroxymethylation of Aldehydes; II. Synthesis of a Novel Bicyclic Amine Organocatalyst,"* March 8, 2010.

Dr. Soumik Biswas (Rutgers University) *"Dehydrogenation and Olefin Isomerization Catalyzed by Pincer-Iridium Complexes, Metathesis of Alkanes from Selectivity and Mechanistic Standpoints,"* March 9, 2010.

Professor Serena DeBeer George (Cornell University) *"X-ray Core Spectroscopy as a Probe of Biological and Chemical Catalysis,"* March 15, 2010.

Meghan Clark (University of Rochester) *"Hydroformylation Using Biphasic Catalysis,"* March 18, 2010.

George Arab (University of Rochester) *"Platinum-Catalyzed Amination of Allylic Alcohols,"* March 19, 2010.

Shujing Wang (University of Rochester) *"Ultrafast Spectroscopy of Single-Chirality Single Walled Carbon Nanotubes,"* March 29, 2010.

## ANDREW S. KENDE DISTINGUISHED LECTURE

Professor F. Dean Toste (University of California, Berkeley)

I. "Development and Application of Gold(I)-Catalysts for the Organic Synthesis," March 31, 2010.

II. "Catalysis with Metal-Heteroatom Bonds," April 1, 2010.

III. "Enantioselective Reactions of Pi-Bonds: New Concepts and Catalysts," April 2, 2010.

### APRIL 2010

## SEYMOUR ROTHCHILD LECTURE SERIES

Professor Robert Crabtree (Yale University)

"Oxidation of Alkyl CH Bonds and of Water with Mn and Ir Catalysts," April 5, 2010.

Sangmin Lee (University of Rochester) "A New Thermal Deposition Boat: Development and Performance Analysis," April 6, 2010.

Dr. Sasa Zaric (University of Pennsylvania)

"Optical/Electrical Properties and the Applications of Carbon Nanotubes," April 7, 2010.

Eric Theiste (University of Rochester) "Steven's

Rearrangement: An Ammonium/Sulfonium 1,2 Rearrangement," April 9, 2010.

Helen H. Wei (University of Rochester) "Towards Synthesis of Nonblinking Quantum Dots," April 9, 2010.

Professor John Asbury (Pennsylvania State University) "Pathways to More Efficient Organic Solar Cells: What We Can Learn by Watching Electrons Move in Real Time," April 12, 2010.

James M. Hart, Jr. (University of Rochester)

"NMR-Assisted Prediction of RNA Secondary Structure," April 14, 2010.

Derek Ryan (University of Rochester) "Design and Optimization of Antimicrobial Peptide Derivatives and Their Potential as Therapeutic Agents," April 16, 2010.

Professor F. Akif Tezcan (University of California, San Diego) "Inorganic Control of Biological Self-Assembly," April 19, 2010.

Jesse Kleingardner (University of Rochester)

"Electronic Structure of Photosynthetic Reaction Centers from Photo-NMR Techniques," April 20, 2010.

Indee Dela-Moss (University of Rochester)

"Using Oligonucleotide Hybridization to Probe RNase P Structure," April 22, 2010.

Leslie Ofori (University of Rochester)

"Peptidomimetic Inhibitors of Histone Deacetylase (HDAC)," April 23, 2010.

Professor Niels H. Damrauer (University of Colorado)

"Controlling Excited-State Energy Conversion in Metal Complexes and Solar-Cell Materials Through Pulse Shaping and Molecular Structure," April 26, 2010.

Wesley Asher (University of Rochester)

"Development of a Heme c Fusion-Tag for Protein Affinity Purification and for Monitoring Protein Unfolding by Ensemble and Single Molecule FRET," April 27, 2010.

Professor Peter T. Wolczanski (Cornell University)

"Synthesis and Applications of (smif)MX Complexes and Other Azaallyl Systems," April 29, 2010.

Tulaza Vaidya (University of Rochester)

"The Development of Photoredox SOMO Catalysis Using Metal Chromophores," April 29, 2010.

Professor Richmond Sarpong (University of California, Berkeley)

"Strategies and Tactics Inspired by Complex Natural Products," April 30, 2010.

### MAY 2010

Professor Alan Smrcka (University of Rochester)

"Small Molecule Modulation of Protein-Protein Interactions in G Protein Signaling," May 7, 2010.

Dr. Bradford Berk (University of Rochester)

"Genetics of Vascular Remodeling," May 7, 2010.

Professor Rudi Fasan (University of Rochester) *"Molecular Discovery with Engineered P450 Enzymes,"* May 7, 2010.

Professor Charles Thornton (University of Rochester) *"Antisense Therapeutics for Genetic Disease: New Luster on Old Magic Bullet,"* May 7, 2010.

Professor Stuart Schreiber (Harvard University) *"Relating the Genetic Features of Cancers to Drug Efficacies Using Small-Molecule Probes,"* May 7, 2010.

Professor Paula Diaconescu (University of California, Los Angeles) *"Reactions of Heterocycles with Electrophilic Ferrocene-Diamide Complexes,"* May 10, 2010.

Jenneke Jalink (University of Rochester) *"Vertically Aligned Carbon Nanotube Membranes for Solar Hydrogen Production,"* May 12, 2010.

Ruja Shrestha (University of Rochester) *"Current Knowledge of the Key Intermediate for Palladium-Catalyzed C-H Bond Functionalization Reactions,"* May 14, 2010.

James Morris (University of Rochester) *"Heterometallic Chemistry,"* May 21, 2010.

Ria Swanekamp & Jennifer Ciesielski (University of Rochester) *"I. Enantioselective Methods for the Synthesis of Amino Acids; II. Part I: Scope and Limitations of a Beta-Iodoallenolate Cyclization, Part II: Progress Towards the Total Synthesis of Phomactin A and Phomactin D,"* May 26, 2010.

## JUNE 2010

Biological Chemistry Cluster Retreat Guest Speakers: Scott Feller (Wabash College) and Peter Moore (Yale University) *See pg. 23 for complete description of seminar titles and events.* June 9-10, 2010.

# Distinguished & Special Lectures



<sup>1</sup> **Barry M. Trost** Victor J. Chambers Memorial Lecture (September 2009)

<sup>2</sup> **Carolyn R. Bertozzi** Harrison Howe Lecture (October 2009)

<sup>3</sup> **Kenneth N. Raymond** Hutchison Memorial Lecture (October 2009)

<sup>4</sup> **F. Dean Toste** Andrew S. Kende Distinguished Lecture (April 2010)

<sup>5</sup> **Robert Crabtree** Seymour Rothchild Lecture (April 2010)



## NEWS FROM THE ADMINISTRATIVE STAFF:

**KAREN S. DEAN** is now in her sixth year in the Department of Chemistry as Administrative Assistant to the Chair and overseeing the day-to-day running of the Department as a whole. In this role, Karen also supports the Chair of the Faculty Recruiting Committee, manages the employment



and immigration requirements for the Department's postdoctoral research associates, supervises the administrative staff, and plays a strong role in supporting the congenial team spirit

within the Department. Two Labrador Retrievers who manage, supervise and contribute daily to the high quality of her life, have recently adopted Karen.

**DONNA J. DOLAN** is a long time staff member in the Department of Chemistry. She is currently beginning her twenty-third year in Chemistry, now serving as departmental receptionist. In this role, Donna continues to provide support for purchasing in the Chemistry Business Office, and organizes the departmental distinguished speakers program, while providing assistance to faculty and managing the Chemistry Department's main office.

**KENNETH SIMOLO (PH.D. '85)** this year celebrates his twenty-third 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.

**DEBRA HARING** bid a very fond farewell to the Chemistry Department on February 1, 2010 to pursue a new position in the School of Arts, Sciences, and Engineering. Debra is now Assistant Dean of Grants and Contracts for AS&E, where she is developing an office which provides extensive pre-proposal grant support to faculty and staff across a broad range of departments and programs representing all the Humanities, Social Science and Science disciplines at UR. She also serves as an additional resource for faculty and administrative staff for pre- and post-award compliance, and as a liaison with the Office of Research and Project Administration and Foundation and

Corporate Relations at the University. Debra worked in the Chemistry Department for ten years, first as administrative assistant to Shaul Mukamel and later as development administrator for Chemistry. The expertise and 'best practices' that Debra gained during her years in the Chemistry Department inform her new role at the College, and she



remains in close contact by assisting with multi-departmental grants involving Chemistry faculty. 2009-10 was a fantastic year, both personally and professionally for Debra. In addition to the exciting promotion to the Deans' Office, Debra was honored last year with the Witmer Award for Distinguished Service. The award provides University-wide recognition to a select number of staff members for careers characterized by outstanding and sustained contributions to the University. Debra is grateful to Chair, Bob Boeckman and Chemistry faculty, who nominated her for this distinction. On a personal note, Debra and her family celebrated her eldest daughter's wedding last August. The wedding took place in her second homeland, Israel, and the entire extended family traveled together to Israel for the first time since their departure in 1997.

**TERRI CLARK** is just starting her third year here in the Chemistry Department as Undergraduate Studies Program Coordinator and Course Administrator and recently moved offices to B19A (come visit anytime!) She also assists faculty in pre-proposal grant preparation, working

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closely with both Debra Haring, now in the Dean's Office, and Lory Hedges, Debra's replacement in the department. What has been especially fun over the past two years, is getting to know the undergraduate chemistry majors and watching their progress towards graduation. This spring, Terri received the Sandra Beach Memorial award for outstanding service to the Department. Terri and her husband travel two or three times each year back to the west coast where their children reside in either California or Washington.

Our Graduate Studies Coordinator, **ROBIN COOLEY**, has now been with the Department for six 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 a large number of prospective graduate students. This past year, the attendees had a great time getting to know one another at "Casino Night," followed by another day of touring Chemistry's facilities, meeting with faculty, and socializing with our current graduate students in Rochester. Once visitation is over, Robin begins the tasks of preparing for the busy week of Orientation for the incoming graduate students. Recruitment efforts were very successful and Chemistry welcomed a new class of sixteen first-year students for the 2010-2011 academic year.

**LORY HEDGES** is our newest addition in the department, starting in the Development Admin and Alumni Relations position in February. She is supporting the faculty on grant and award submissions as well as coordinating Alumni Relations in all its various forms. She is busy learning the ropes of all the events and tasks that go through the office as well as on several sections of the website. She is grateful to Debra Haring and all the department folks who have been helping her. Lory comes to the Chemistry Department from having her own business as a technical grant writer. Her educational background is in industrial engineering with a BSIE from Purdue University. She spent many years at Bausch & Lomb in the manufacturing area, implementing new products and processes. She and her partner, Paul Taylor, have just purchased a home in the UR area and Lory walks to Hutchison Hall. They both love to travel and especially enjoy day trips in the area. Lory enjoys cooking and gardening, is an avid quilter, and volunteers in the Compeer Quilting Bee.

**MARGUERITE WESTON**, Assistant to Faculty, has been with the Department of Chemistry for fifteen years. She coordinates the Chemistry Seminar Program and produces the online seminar schedule each month. Marguerite also coordinates select special events, assists with various projects, and provides support to numerous faculty members. Marguerite assists



Professor Thomas Krugh with the many administrative details of Chemistry's National Science Foundation supported annual summer research program for undergraduates (REU), including preparation of the competitive renewal proposals for each three-year period and annual reports. The Department was again awarded a three-year renewal by NSF for its REU Program which attracts approximately 125 applications each year from undergraduates across the nation and the University of Rochester.

**ELLY YORK**, who joined the Chemistry Department in November of 2006, works as a teaching assistant in the undergraduate laboratories and is the sole TA for the summer sessions of the general chemistry laboratory. Elly also assists with safety inspections in the Department, as well as working part time in the Chemistry stockroom. Elly is a graduate of Alfred University and has clinical work experience, having previously worked in several veterinary clinics prior to coming to UR. She also recently completed a Master's degree in education and was married last year. Elly and Brandon have just bought their first house. Congratulations!

## NEWS FROM THE EDITORIAL OFFICES OF JOURNALS OF THE AMERICAN CHEMICAL SOCIETY:

**KIRSTIN CAMPBELL** oversees the staff of *Inorganic Chemistry* as Coordinating Editor. Out of 44 journals in their category, *Inorganic Chemistry* is once again the most-cited journal in inorganic chemistry with a record 79,450 total citations in 2009 and an impact factor of 4.657, its highest ever. The Rochester office, the main office of the journal, overseen by Editor-in-Chief Richard Eisenberg, handled over 2,553 manuscripts in 2009. *IC* is one of the few ACS journals featuring issues with a changing cover, being published twice a month. *Inorganic Chemistry* is in preparatory stages of kicking off the 50-year celebration of the journal in 2011. On a personal note, Kirstin has been busy at home, enjoying and working with three new additions to her equine family. April 2009 produced a percheron colt named Willie Just Do-It (Willie), and the following April his younger full brother Rorschach (Norman) arrived. In July 2010, an Oldenburg filly named Senona made her appearance into the world. Percheron are an imported French draft breed, and aren't very common in the US. Oldenburg are an imported German warmblood breed,



*Kirstin Campbell with Willie*

and Kirstin looks forward to charting their development.

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

**VALERIE FITZHUGH** has been working as an editorial assistant in the Department of Chemistry for almost nine years. She served on the journal staff of the *Inorganic Chemistry* EIC office and *The Journal of Organic Chemistry* before assuming her current position as Editorial Assistant to Associate Editor William D. Jones for *The Journal of the American Chemical Society (JACS)* eight years ago. Interacting with authors, editors and reviewers in this role has been an enriching experience for Val. She continues to find the fast pace of the *JACS* editorial office challenging and interesting. Processing the 460+ submitted manuscripts to editorial decision and/or production, as well as assisting authors of cutting-edge science publish their work, has made her career a very satisfying and rewarding one. *JACS* is the premier, state-of-the-art venue for the publication and broad dissemination of first-rate, fundamental research in all of chemistry, both in the core areas and at the interface of chemistry and biology, neurochemistry, materials, and single molecule chemistry. In 2009, *JACS* set the bar ever-higher as the most-cited journal in chemistry with a record 351,813 total citations, an increase of 10.5% over 2008, maintaining better than twice the total citations as *Angewandte Chemie* (164,626 total cites for an 18% increase). *JACS* also continues to publish more research than any other journal in the field, with 3,332 articles in 2009, a slight increase over 2008. This is evidence of another great year for the journal, staying ahead of the pack and making a significant contribution to chemistry and the related sciences.

**DAWN MURPHY** is starting her third year as an editorial assistant to both the *Journal of Organic Chemistry (JOC)* and *Journal of the American Chemical Society (JACS)*. Dawn likes the diversity and challenge of working in two different journal offices, assisting Terrell Samoriski and Valerie Fitzhugh in their respective roles as editorial assistants. In her previous employment, Dawn also worked in electronic publishing for the *American Economic Review* at the University of California, San Diego. Dawn continues to teach art history as an adjunct professor at Monroe Community College where she enjoys interacting with students. After living in Southern California for many years Dawn spends much of her spare time taking in the many cultural and family events Rochester and surrounding area has to offer and really appreciates being close to family and friends. This year she vacationed with her two daughters in Tybee Island and Savannah, Georgia.

**TERRELL SAMORISKI** completed her sixth year as Editorial Assistant for *The Journal of Organic Chemistry (JOC)*. She works closely with Professor Robert K. Boeckman, Jr., Associate Editor for *JOC* and continues to enjoy her work in scientific publishing. Terrell also assists with scientific proofreading for departmental documents, such as proposals, manuscripts and brochures. The *JOC* publishes original contributions reporting novel, important findings of fundamental research in all branches of the theory and practice of organic and bioorganic chemistry. Due to the increase in submissions and the implementation of the web-based submission procedure, the journal expanded to include an associate editor's office in Europe and China. According to the most recent ISI statistics, *JOC* remains number one in total citations in organic chemistry (over the number two journal, *Tetrahedron Letters*), with 92,992 cited for the year 2009, translating to an increase of 7.4% in total citations since 2008. The journal publishes

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*Terrell Samoriski and Kirstin Campbell*



both shorter articles (Notes) and lengthier ones (Articles), the covers of which continue to be a highly desired forum for authors to showcase art relating to their manuscripts.

## NEWS FROM THE SCIENTIFIC AND TECHNICAL STAFF:

**TERRY (TED) O'CONNELL** started his twenty-eighth year with the Chemistry Department and enjoys his position as Director of Technical Operations. He is responsible for new equipment installations and any building renovations. In the past year, the department acquired and installed over \$2,000,000 worth of research instrumentation, including: a Bruker EMX-Plus EPR spectrometer, a Thermo LTQ Velos Ion Trap LC/MS, a Bruker Fourier Transform Mass Spectrometer (FTMS); a Perkin Elmer 2400 CHN/S Analyzer, and a Bruker Autoflex III MALDI-TOF. He works closely with Senior Lab Engineer **PETE SERRINO** and Research Scientist **SANDIP SUR**, as well as **ERIC LOBENSTINE** and **RAY TENG**.

**ERIC LOBENSTINE (PH.D. '81)**, Manager for Computers and Network spent a significant amount of his time this past year working with a University IT committee on a major upgrade for the email service for both graduate students and postdocs, to insure that our needs would be met. This transition went (reasonably) smoothly at the end of May; so many students were eager to play with the new system that it took almost a week to move all the users' emails! Eric is very happy to announce that Hutchison Hall now has wireless network access. Since it was one of the last academic buildings on the River Campus without ubiquitous wireless access, Eric has been pushing hard for this service for several years now. On a personal note, Eric's older Brian graduated *Magna Cum Laude* in May, with a B.A. in Financial Economics and minors in Chemistry and English. After an internship this summer at Global Crossing, Brian is attending the Simon School in the fall

*Eric Lobenstine with son, Brian, and wife, Jeanne*



to work on his M.B.A. Ethan, Eric's younger son, now a Senior had a great summer working as an Orientation Leader for the 1200+ students who arrived for the 2010-2011 academic year.

**RAY TENG (B.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 2009, minor renovations in Hutchison Hall were undertaken: Room 468 was converted to a computer lab, B25 was renovated for a new Bruker Low Temperature EPR, and office space (431) was renovated for our new faculty hire, Oleg Prezhdo. 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 to which he has now added "the college search" for D3 soccer schools.

Once a chemist has synthesized a new molecule, he or she needs to "characterize" it in order to prove to the scientific community that it really exists. Two of the most important and trusted means of characterization for solid samples are single crystal X-ray crystallography and combustion elemental analysis. The former technique determines the composition of one crystal (like a sugar or salt crystal) and provides the chemist with the identity and arrangement of atoms in the sample. The latter technique involves burning a portion (about 2 mg) of the bulk solid sample and measuring the amount of carbon dioxide, water, and nitrogen to provide the chemist with the absolute percentages of carbon, hydrogen, and nitrogen in the sample. Our crystallographer, **BILL BRENNESEL**, has been busy with the management and operation of facilities dedicated to those two techniques. The X-ray Crystallography Facility continues its high turnout of results with, on average, a new sample run daily. In addition, undergraduate students get hands-on training as part of the inorganic techniques course, CHM 234, and graduate students learn the theory and full operation of the instrumentation in CHM 417. Students who have taken CHM 417 are officially trained users of the facility and can examine their own research samples. The new CENTC Elemental Analysis Facility, provided by a grant obtained through Professor William Jones and CENTC (Center for Enabling New Technologies through Catalysis), has been running for nearly six months now. The instrumentation includes the combustion analyzer, a microbalance, and a high-end glovebox used to prepare samples that react with the oxygen or water in air. Despite the synthetic research community's routine use of this technique, it is surprising that we are one of the few universities to have a facility on site. The in-house nature of the facility not only eliminates shipping

costs, but allows for immediate results without having to pay exorbitant fees for rush service. And with Bill Brennessel (“Dr. X-ray”) as the sole instrument operator, there is an inherent consistency that is not realized in commercial facilities.

Chemistry faculty and students are aided in their research by numerous invaluable instructional, scientific, and technical staff. The Department appreciates the efforts and contributions of senior scientists **PAUL MERKEL** (Dinnocenzo group), **JAN TÖKE** (Schröder group), as well as instructors **DAVID HICKEY (PH.D. '85)** and **BRUCE TODER (POSTDOC. '82)**. Dr. Hickey and Dr. Toder oversee our undergraduate labs for general and organic chemistry during the academic year and in the summer, teach CHEM 131 and CHEM 203/204 (plus labs), respectively.

## NEWS FROM THE SCIENCE LIBRARY:

**SUE CARDINAL**, Chemistry Librarian from the Carlson Library reports that the University has permanent access to the ACS journals online. We’ve also added online access to back issues of *Angewandte Chemie* and *Chemische Berichte*. We are moving seldom used print journals to a storage facility and next year will convert the freed space into student work space. We spend a few hours each week in a nearby cafe answering science reference questions.

## NEWS FROM THE BUSINESS OFFICE:

The Business Office continues to provide service to faculty, staff and students on all financial matters such as payroll, reimbursements, purchases, preparation of grant budgets and monitoring grant expenditures. **DORIS WHEELER**, Business Office Manager since 2002, is happy to report that the Business Office is once again fully staffed. **ANNA KUITEMS** is the newest addition to the Business Office Staff transferring from Eastman School of Music where she was a staff accountant for five years. Before Eastman, Anna was in Accounts Payable at the Towne House. Her husband Russell and she moved back to the Rochester area after 26 years and have lived in many places throughout the U.S. (Austin, TX, Dayton, OH, Los Angeles and Burlington, VT). While living in Burlington, Anna worked for the University of Vermont. Her last position was in Molecular Physiology and Biophysics as a Financial Assistant. Anna and Russell have two sons and a daughter. Anna is responsible for reconciling grant ledgers, P-card management and graduate student payroll, and as backup

for Randi’s position. Anna looks forward to working with the faculty, staff and students in the Chemistry Department. The Business Office staff also consists of three additional members with valuable experience. **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. This year Paul celebrated a milestone anniversary – 25 years of service to the Chemistry Department. Congratulations and thank you for the many years of valued service to the University!

*Clock Tower in Dandelion Square*





## DID YOU KNOW...

...that the University of Rochester ranked number thirteen among the nations top 25 “best neighbor” colleges and universities in 2009? The “Saviors of our Cities: A Survey of Best College and University Civic Partnerships,” was first published in 2006. Academic institutions are selected based on their positive impact on their urban communities and include both commercial and residential activities such as revitalization, cultural renewal, economics, and community service and development.



# Departmental Funds

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

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

## Chemistry Alumni Research Fund

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

## Marshall D. Gates, Jr. Chair in Chemistry Fund

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

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

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

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

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

## Richard S. Eisenberg

### Chemistry Endowment Fund

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

## Magomedov-Shcherbinina Memorial Fund

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

## Distinguished Lectureship Funds

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

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

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

*W. Albert Noyes, Jr. Memorial Lectureship* honors Professor Noyes, former Chairman of the Department, Dean of the Graduate School and Dean of the College of Arts and Science.

## I wish to contribute to the following fund:

Chemistry Alumni Research Fund

Other - Please specify \_\_\_\_\_

My gift is in honor of \_\_\_\_\_ (see page 7 for example)

## Contact Information:

NAME \_\_\_\_\_

ADDRESS \_\_\_\_\_  
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## Degree Information:

*Year degree(s) received from the Department*

B.A. \_\_\_\_\_

M.S. \_\_\_\_\_

B.S. \_\_\_\_\_

PH.D. \_\_\_\_\_

ADVISOR \_\_\_\_\_

Please send your contribution and this form to: Lory Hedges, 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](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:**

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

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

### Contact Information:

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### Degree Information:

*Year degree(s) received from the Department*

**B.A.** \_\_\_\_\_

**B.S.** \_\_\_\_\_

**M.S.** \_\_\_\_\_

**PH.D.** \_\_\_\_\_

**ADVISOR** \_\_\_\_\_

**LATEST NEWS**

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**NEWSLETTER COMMENTS**

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