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Faculty and Staff

FACULTY

PROFESSORS OF CHEMISTRY

Robert K. Boeckman, Jr. Kara L. Bren Joseph P. Dinnocenzo **Richard Eisenberg** James M. Farrar Rudi Fasan Alison J. Frontier Joshua L. Goodman Patrick L. Holland William D. Jones, Jr. Todd D. Krauss Thomas R. Krugh David W. McCamant Bradley L. Nilsson Misha Ovchinnikov Lewis J. Rothberg W. Udo Schröder Harry A. Stern Ching W. Tang Douglas H. Turner Daniel J. Weix

PROFESSORS EMERITI

Frank P. Buff John R. Huizenga Jack A. Kampmeier Andrew S. Kende Robert W. Kreilick John S. Muenter William H. Saunders, Jr.

RESEARCH PROFESSORS

Esther M. Conwell Samir Farid

SENIOR SCIENTISTS

Paul Merkel Jan Tõke

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Arlene Bristol Kirstin Campbell Terri Clark Robin Cooley Karen Dean Marcia Eisenberg Valerie Fitzhugh Dawn Murphy Terrell Samoriski

ASSISTANT TO FACULTY Marguerite Weston

BUSINESS OFFICE

Diane Evans Randi Shaw Diane Visiko Doris Wheeler

SECRETARIES Donna Dolan

STOCKROOM

Paul Liberatore Elly York

TECHNICAL STAFF

William Brennessel William Herkstroeter Eric Lobenstine Terry O'Connell Peter Serrino Sandip Sur Ray Teng

UNDERGRADUATE LABORATORY INSTRUCTORS

David Hickey Bruce Toder

CHEMISTRY LIBRARIAN

Susan Cardinal

From the Chair



Greetings to all Department of Chemistry Alumni! We enjoyed a busy and productive 2008-2009 academic year in the Department and at the University. As I enter my seventh 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 academic year.

Inevitably, the economy had an impact upon all of us, and the University of Rochester is no exception in feeling the stress from the economic events of the last year. I am proud to say that it appears Rochester will weather this crisis far better than many of our peer institutions. The University has made sustaining the quality and distinction of our undergraduate programs one of its highest priorities and is devoting a considerable proportion of available resources to help students, and their families, weather these difficult economic times with respect to achieving a college education.

In June 2009, President Seligman reported that the endowment had lost approximately 20% (after withdrawals for spending) and dropped from about \$1.7 billion on June 30, 2008 to approximately \$1.35 billion on May 31, 2009. The University responded promptly to the economic crisis last fall by significantly reducing endowment payout with various cost saving measures and putting some major projects on hold. However, loss in the endowment, while serious, is only a part of the financial equation for most schools that make up the University. Four types of financial support drive our academic programs: tuition, sponsored research, gifts, and endowment payout. Most of UR's academic divisions in the College of Arts, Sciences and Engineering, including the Chemistry Department, are tuition driven. The very good news is that this was a record year for applications to the undergraduate program at the College, and the Chemistry Department anticipates that

a proportionate number of incoming Freshmen will participate in the chemistry curriculum. Furthermore, despite an ailing economy, UR Chemistry alumni have remained constant in their generous support of the Department, and the Department is 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 reached nearly four 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 hope that better days are ahead and are gratified 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, and will continue to apply, for federal funding under the auspices of the American Recovery and Reinvestment Act, as well as other federal and state programs. Last year our 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 and other Young Investigator awards.

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 grow to 24-26 over that period, both to accommodate increasing enrollments as well as 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. Although Chemistry was not selected as one of the departments permitted to make a faculty hire this year, University leadership is aware that enlisting vigorous young and mid-career faculty, who excel in research and teaching, is critical going forward. Ultimately, new research initiatives, such as those in systems biology, nanotechnology, renewable energy (particularly fuel cell and hydrogen production), and identification of gene function, coupled with the expected growth in the student body, and a maturing demographic among our senior faculty, will precipitate hiring of new faculty. Proactive effort to retain faculty, in an era of increased mobility, also remains a critical focus.

Chemistry faculty received several notable awards this year, the details of which you will read in this Newsletter. Esther Conwell was the recipient of an Honorary Doctorate of Science from SUNY Geneseo. Jack Kampmeier and his colleagues in chemical education and Peer-Led Team Learning, David Gosser and Pratibha Varma-Nelson received the ACS NE Section's Jack Flack Norris Award for Outstanding Achievement in the Teaching of Chemistry last November. Doug Turner and Lewis Rothberg were awarded University Provost's Multidisciplinary Awards in 2008 and Todd Krauss was a recipient of this award in 2009. Dave McCamant was awarded the NSF CAREER award, Bill Jones was awarded the ACS Arthur C. Cope Scholar Award, the University's Edward Peck Curtis Award for Excellence in Undergraduate Teaching, as well as a Fellowship Award from the Japan Society for the Promotion of Science. Rich Eisenberg was elected to the American Academy of Arts and Sciences and I was honored with the William H. Riker University Award for Graduate Teaching. Rich Eisenberg and I were also recently elected to the 2009 class of Fellows of the American Chemical Society. This kind of recognition helps to sustain our efforts to recruit and retain high quality faculty and students, and enhances 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 record 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.

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

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 the basement to accommodate a Bruker FTMS. Hutchison Hall 421 was converted into a user facility housing microwave and hydrogenation apparatus. In the near future, we plan to seek an upgrade to our ESR and Mass Spectroscopy facilities, and are working with University leadership to seek NSF funding to upgrade ventilation and electrical systems in our building. Through the generous gifts of our alumni and other University and unrestricted funds, we will continue the staged renovation of Chemistry's research laboratories over the next several years.

For many years we have aspired to grow our graduate program. I am happy to report that this year Chemistry has experienced significant growth with regard to our incoming first-year graduate students: a record number of 31 graduate students entered our doctoral program this fall, bringing the total

number of graduate students in the Department of Chemistry to approximately 120.

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

Meliora and best wishes to all for a successful and happy year in 2009-2010.

tobet t. Boeckman

Bob Boeckman

Hutchison Hall



Includes donations received between July 2008 and June 2009.

GIFTS OF \$50,000+

Dorothy B. Rosenberg-Passer (B.A. '48, M.A. '51)

GIFTS OF \$12,000 - \$49,999

Pawel Fludzinski (M.S. '80, Ph.D. '83, Postdoc '83) John E. (M.S. '75, Ph.D. '78) and Judith A. Mills Yuh-Geng (M.S. '75, Ph.D. '77) and Margaret H. Tsay

GIFTS OF \$5,000 - \$11,999

Robert A. Bourque (M.S. '77, Ph.D. '80) F. Hal (M.S. '80, Ph.D. '84) and Sheila Ebetino Louis N. Jungheim (Postdoc '81) Steven J. Lee (Ph.D. '73) Wuu-Yong (Ph.D. '74) and Margaret (M.S. '74, Ph.D. '76) Wu

GIFTS OF \$1,000 - \$4,999

Edwin D. Becker (B.S. '52) Karen Hill Brown (B.A. '61, Ph.D. '72) Barbara J. Burger (B.S. '83) Joseph (Ph.D. '72) and Theresa Chu Walter Cooper (Ph.D. '57) Peter and J. Robin (M.S. '87, Ph.D. '92) Cowdery-Corvin Richard and Marcia Eisenberg Samir Farid Richard A. (B.A. '77) and Lori C. Josephson (B.A. '78) Jiong Lan (Postdoc '02) Norman P. (B.A. '52) and Mary G. Neureiter Thomas J. Perun (Ph.D. '63) David H. Presky (B.S. '78) Elliot (B.S. '70, Ph.D. '75) and Laura Richman David N. (M.S. '74, Ph.D. '76) and Paula Ridge Pauline SanFilippo (Ph.D. '84) Seymour Siwoff Joseph P. Smith (B.S. '72) Steven M. (Ph.D. '67) and Nancy E. (B.A. '64) Weinreb

GIFTS OF \$500 - \$999

Prudence K. Bradley (M.S. '84, Ph.D. '88) Joseph P. Dinnocenzo John I. Fitzmorris (B.S. '64, M.S. '71) Kenneth F. Greenough (Ph.D. '60) Paul Hebeisen (Postdoc '83) Thomas A. Henderson (M.S. '83, Ph.D. '86) Norman A. Leister (Ph.D. '58) Lanny (M.S. '74, Ph.D. '77) and Diane Liebeskind Jack L. (Ph.D. '70) and Jo Ann H. Richards Thomas N. Thompson (B.S. '77, M.S. '81, Ph.D./M.D. '85) Joseph Weinstock (Ph.D. '52)

GIFTS OF \$250 - \$499

Edward A. (Ph.D. '63) and Virginia B. (Ph.D. '64) Caress Chiu S. Chang (Ph.D. '71) Thomas J. Hall (Ph.D. '53) David J. Hart Roy A. Leckonby (Ph.D. '76) Ronald M. Levinson (B.S. '56) William J. Linn (Ph.D. '53) Kun Liu (M.S. '93, Ph.D. '95) Margaret Logan (M.S. '72, Ph.D. '82, Postdoc '88) William E. Lovett (Ph.D. '56) Roger (Postdoc '73) and Patricia Mader Guido V. Marinetti (B.S. '50, Ph.D/M.D. '53) Thomas A. Montzka (Ph.D. '62) Matthew R. Robinson (B.S. '98) Suzanne Stokes Stimler (Ph.D. '58) James R. (M.S. '84, Ph.D. '88) and Patricia V. Tata (M.S. '84) Sanford T. (Ph.D. '63) and Margaret Young

GIFTS OF \$100 - \$249

Sylvia L. Betcher (B.A. '70) Richard P. English (B.S. '65) Robert P. Frankenthal (B.S. '52) William P. Hauser (Ph.D. '61) Scott M. Kampmeier and Julie A. Eklund Frederick D. Lewis (Ph.D. '68) George W. (Ph.D. '50) and Doris W. (B.A. '50) Luckey Paul C. (M.S. '77, Ph.D. '79) and Stella K. Naegely Joseph D. (Ph.D. '45) and Mary L. Overman Brian R. Rohrs (B.S. '83) Noel (Ph.D. '68) and Anne (Ph.D. '69) Turner W. Bernard Wargotz (Ph.D. '55) Linfeng Xie (M.S. '87, Ph.D. '90) Min Zhong (Ph.D. '99)

OTHER GIFTS

Wesley E. Bentz (Ph.D. '71) Noal (B.S. '59) and Ann B. Cohen Ronald H. Micheels (B.S. '72) Albert H. Soloway (Ph.D. '51) Samuel S. Stradling (Ph.D. '64) Kumiko E. Tanaka (B.A. '07) Dorothy Toomey Stephen T. (M.S. '93, Ph.D. '97) and Michelle L. (M.S. '94, Ph.D. '98) Wrobleski

CONTRIBUTIONS IN MEMORY OF...

Moses Passer (B.S. '45) Dorothy B. Rosenberg-Passer

Magomedov-Shcherbinina Family

Joseph P. Dinnocenzo Samir Farid David J. Hart

Carl A. Whiteman, Jr. (B.S. '50 in Physics)

Joseph P. Smith Dorothy Toomey

CORPORATE CONTRIBUTIONS...

Abbott Laboratories Bristol-Myers Squibb Company Chevron Corporation E.I. du Pont de Nemours & Company Eli Lilly & Company Foundation ExxonMobil Foundation IBM Corporation Johnson & Johnson Company Novartis Pharma AG Shell Oil Company Foundation Texas Instruments, Inc. Thermo Fisher Scientific Laboratory



Alumni News

ERWIN KLINGSBERG (PH.D. '44) presented a lecture on August 17, 2008 at the 236 National ACS meeting in Philadelphia entitled "Three ACS Questions" under the auspices of the ACS Division of the History of Chemistry. Dr. Klingsberg worked at American Cyanamid's Bound Brook Laboratory from 1946 until 1981, rising to the rank of Research Fellow. He is author and inventor of over 75 publications and patents, has lectured on his work in many parts of the world, and has held a number of visiting professorships in the U.S. and abroad. Now retired, he resides in Washington, DC and continues to do research in the history of chemistry.



EDWIN D. BECKER (B.S.

'52) was elected to the inaugural class of Fellows of the American Chemical Society in 2009. Established in 2008, the ACS Fellows program recognizes those scientists who have distinguished themselves in multiple areas, including the promotion of science, the profession, and service to the American Chemical Society. Dr. Becker has spent the major part of

his career since 1955 at the National Institutes of Health near Washington, DC. He has been Chief of the Molecular Biophysics Section, 1961-72; Chief of the Laboratory of Chemical Physics, 1972-80; Associate Director for International Research, 1979-81; Associate Director for Research Services, 1980-88; Chief of the NMR Section in the Analytical Chemistry Laboratory, 1988-98; and Scientist Emeritus, 1998 to present. He is internationally known for his research in molecular spectroscopy and nuclear magnetic resonance (NMR), and for his three books on NMR.

ROBERT P. FRANKENTHAL (B.S. '52) received the ECS Edward Goodrich Acheson Award in 2008. After leaving Rochester, he earned his Ph.D. in analytical chemistry from the University of Wisconsin (1956), where he was a Procter and Gamble Fellow in 1954-1955. Thereafter, he joined the Applied Research Laboratory of U.S. Steel Corp. and in 1960, he transferred to U.S. Steel's E. C. Bain Laboratory for Fundamental Research, where he conducted research on the passivation and localized corrosion of iron and ferrous alloys and the application of new surface analytical and electrochemical techniques to corrosion research. In 1972, he joined Bell Laboratories to study the corrosion and passivation of metals and the protection and reliability of electronic materials and devices. His research has resulted in more than 100 publications and eight patents. In 1983, he received the Distinguished Technical Staff Award for Sustained Achievement from Bell Laboratories and has been the recipient of numerous other honors; He was elected an ECS Fellow in 1995 and an ECS Honorary Member in 2003. He received the H. H. Uhlig Award of the ECS Corrosion Division in 1989 and was honored by the Division with a symposium and proceedings volume, "Corrosion Science: A Retrospective and Current Status in Honor of Robert P. Frankenthal" in 2002. He was also named a Fellow of NACE International in 1994 and received that society's Willis R. Whitney Award in 1997. Dr. Frankenthal has also been active in various elected and appointed positions in other societies, most recently as Editor-in-Chief of the *Journal of Materials Research* (1998- 2001) for the MRS.

WALTER COOPER (PH.D. '57) was the recipient of two tributes this past year commemorating his career-long record of civic engagement. In September 2008, UR's Frederick Douglass Institute for African and African-American Studies awarded Frederick Douglass Medals to two recipients in recognition for their efforts to ensure equal opportunity in education and in the workplace. Walter Cooper, retired research scientist at Eastman Kodak Company, was honored along with David Kearns, retired CEO of Xerox Corporation. Both were presented with the medals at the inaugural Frederick Douglass Dinner at the UR Medical Center by President Joel Seligman. Dr. Cooper is a New York State Regent Emeritus and 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



Walter Cooper Ph.D. '57 and President Joel Seligman

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 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. In another effort to honor Walter Cooper's myriad contributions to the City of Rochester, it was announced later in 2009 by Superintendent Jean-Claude Brizard that a new Rochester public elementary school will soon bear his name. The Rochester Board of Education approved the naming of the school; the Dr. Walter Cooper Academy opens this fall at 353 Congress Ave. "Walter Cooper is a legend and he exemplifies educational excellence," said school board President Malik Evans. "He understands the challenges in education but sends the message of not letting challenges limit ability. His life is an example of that."



SUSAN R. FAHREN-HOLTZ (M.S. '60) was elected to the inaugural class of Fellows of the American Chemical Society in 2009. The ACS Fellows is a new program; the 162 newly elected members in the inaugural class "share a common set of accomplishments, namely true excellence in their contributions to the chemical enterprise coupled with distinctive

service to ACS or to the broader world of chemistry," said Past-President Bruce E. Bursten, who advocated for creation of the program in 2008. Susan R. Fahrenholtz, an adjunct professor at Fordham University and retired chemist from Bell Labs, has championed disadvantaged students during her entire career. In addition to teaching at Fordham, she volunteers with the North Jersey Section Summer Educational Experience for Economically Disadvantaged (SEED) students program, which provides mentors for high school students doing scientific research at various universities. In 2006 she was recognized for this work with the ACS Award for Encouraging Disadvantaged Students into Careers in the Chemical Sciences, sponsored by the Camille & Henry Dreyfus Foundation.

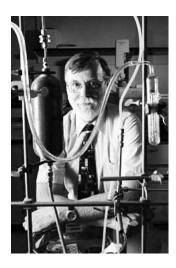
RICHARD ENGLISH (B.S. '65) wrote that one of his fondest memories of the Chemistry Department was Marshall Gates' personal delivery of a birthday cake on his birthday to his freshman dormitory, thanks to a long-standing relationship between Marshall Gates and his father. He also recalled his student days with Jack Kampmeier, although his chemistry career took him in the direction of physical, not organic, chemistry. After leaving Rochester, Dr. English went on to earn a Ph.D. in physical chemistry from MIT. Upon graduation, he moved into the 'real' world of chemistry quickly by working at GE in West Lynn, MA for two years doing applied research. He then relocated to San Jose, CA to join GE's Nuclear Power Group, first as a materials and process engineer and later as a manager of a mechanical design engineering group, designing nuclear fuel elements. The latter part of his industrial career was spent in management roles in the semiconductor capital equipment industry. About eight years ago, he and his wife moved to the San Jose, CA area where he now works remodeling houses and as a part-time career coach, assisting people in career transition.

SUEDEEN G. KELLY (**B.A. '73)** In March 2009, President Barack Obama announced his intention to nominate Suedeen Kelly for Commissioner of the Federal Energy Regulatory Commission. Dr. Kelly has served as a Commissioner at the Federal Energy Regulatory Commission since November 2003. In December 2004, she was confirmed to a second term



that expired June 30, 2009. Previously, she was a Professor of Law at the University of New Mexico School of Law, where she taught energy law, public utility regulation, administrative law and legislative process. She also worked with the law firms of Modrall, Sperling, Roehl, Harris & Sisk in Albuquerque from 2000 through 2003 and Sheehan, Sheehan, and Stelzner from 1992 through 1999. In 2000, Dr. Kelly served as counsel to the California Independent System Operator. In 1999, she worked as a Legislative Aide to U.S. Senator Jeff Bingaman. Prior to joining the faculty of the Law School, Kelly served as Chair of the New Mexico Public Service Commission, which regulated New Mexico's electric, gas and water utilities. She had been a lawyer in the Office of the New Mexico Attorney General and with the New Mexico firm of Leubben, Hughes & Kelly and has worked in Washington, DC, for the Natural Resources Defense Council and Ruckelshaus, Beveridge, Fairbanks & Diamond. Sudeeen Kelly received her B.A. with Distinction in Chemistry from the University of Rochester and a J.D. cum laude from Cornell Law School. She is admitted to the bars of New Mexico and the District of Columbia.

DENNIS CURRAN (PH.D. '79) was elected to the inaugural class of Fellows of the American Chemical Society in 2009. The ACS Fellows is a new program, established in 2008, which recognizes those scientists who have distinguished themselves in the promotion of science, service to their profession, and service to the American Chemical Society. Having joined the faculty of the Chemistry Department at the University of Pitts-



burgh in 1981, Dennis Curran is Distinguished Service Professor and Bayer Professor of Chemistry and the founder of Fluorous Technologies, Inc. The recipient of numerous awards, Prof. Curran has authored over 350 papers, thirty patents and two books, and is renowned for his work at the interface of radical chemistry and organic synthesis. Most recently he has made important contributions to the emerging discipline of fluorous chemis-

try and in 2008, received the ACS Award for Creative Work in Fluorine Chemistry. While a graduate student at Rochester, he completed his doctoral work under the direction of Andrew S. Kende.

CLIFFORD KUBIAK (PH.D. '80) was the recipient of the University of Rochester Distinguished Scholar Award in 2009. This award recognizes alumni with doctoral degrees from UR who have distinguished themselves in their professional fields. The award presentation took place at the 2009 doctoral graduation ceremony at the Eastman Theater on May 16, 2009 in Rochester. Cliff Kubiak is currently the Distinguished Professor of Chemistry and Harold C. Urey Chair of Chemistry at the University of California, San Diego. He was recognized by UR for demonstrating extraordinary creativity in addressing problems of deep fundamental interest in chemistry, and versatility as a scientist to lead the way toward solutions of globally important problems in energy research. He is currently leading his research group in innovative and exciting inorganic chemistry, including ultrafast electron transfer in chemical reactions, the developing field of molecular electronics, and globally important problems in energy research; his work is of interest to a broad cross-section of scientists in the chemistry and physics community. One of the leading authorities on the chemistry of carbon dioxide, his work on this molecule is applicable across a range of energy problems. His current research on the photochemical "splitting" of carbon dioxide to carbon monoxide and oxygen is one of the few energy conversion schemes that pro-



duces a useful chemical fuel precursor (carbon monoxide) from a greenhouse gas (carbon dioxide). Prof. Kubiak was one of the key figures in the field of chemistry who early on recognized the potential of nanotechnology. He is now both a pioneering veteran of the first days of chemical nanotechnology and a modern practitioner applying principles of nanotechnology to energy research. During his graduate student days at Rochester, he completed his doctoral studies under the direction of Richard Eisenberg. He then pursued postdoctoral research in photochemistry from 1980-1981 with Mark S. Wrighton at MIT before joining the faculty at Purdue University. He joined the faculty at the University of California at San Diego in 1998, having served as Chairman of the Department of Chemistry & Biochemistry at UCSD from 2002-2006. He has chaired prominent committees and working groups for the American Chemical Society, and has been the recipient of numerous awards and honors such as the NSF Award for Special Creativity (2008) and has been named Fellow of Japan Society for the Promotion of Science (1996 and 2007) and Alfred P. Sloan Foundation Research Fellow (1987-1991). A dedicated educator and mentor he has received many teaching awards as well.

BRUCE ROTH (POSTDOC-TORAL FELLOW '82) was

named one of the "Heroes of Chemistry" by the ACS in August 2008 at the National Meeting in Philadelphia. Dr. Roth was among 25 unsung scientific heroes who were inducted into the American Chemical Society hall of fame called the Heroes of Chemistry. This recognition honors chemical innovators in industry whose work leads to the



welfare of humanity in a significant way during the past decade. Bruce Roth is best known as the inventor of Lipitor, the cholesterol-lowering medication that is the world's largest selling drug. Dr. Roth first began on the path toward inventing the molecule atorvastatin that became Lipitor in 1982, when he joined the Warner-Lambert/Parke Davis Company in Ann Arbor, Michigan, as part of a project to discover drugs to inhibit the body's production of cholesterol. After synthesizing atorvastatin, he served as the lead discovery chemist who helped shepherd Lipitor through clinical trials. Warner-Lambert merged with Pfizer in 2000 and currently markets the drug; Dr. Roth worked at Pfizer for 25 years, the last seven of which as Vice President of Chemistry. In 2007, he joined Genentech in South San Francisco where he is currently Senior Director of Discovery Chemistry. Michael Varney, a vice president of Genentech who nominated Dr. Roth for the award, termed the invention of Lipitor a "monumental achievement" and says, "Lipitor is currently the largest selling pharmaceutical in the history of mankind, with annual sales of over \$13 billion worldwide. The low density lipoprotein lowering ability of Lipitor has contributed to the reduction of countless cardiovascular events such as heart attacks and stroke. By virtue of its clinical benefit, Lipitor has saved the lives of many people, reduced the pain and suffering of many people, and saved society and the health care system billions of dollars."

MATTHEW SHAIR (B.S. '90) was a recipient of the 2009 Raymond and Beverly Sackler Prize in the Physical Sciences for Chemistry. The research field for the 2009 Sacker Prize was the "Total Synthesis of Biologically Active Natural Products." This year, three young chemists shared the prestigious prize, which is administered by Tel Aviv University: Matt Shair, Phil Baran and Brian Stoltz. The Sackler Prize was shared equally among the three recipients and was awarded to them in person on May 19, 2009, during a one-day symposium honoring the distinguished laureates at Tel Aviv University in Israel. Since his Rochester days, Prof. Shair went on to receive his M.S. from Yale in 1993 and his Ph.D. from Columbia in 1995. He completed postdoctoral research at Harvard in 1997, and since that time has risen through the ranks to tenured Professor of Chemistry and Chemical Biology at Harvard University. The Sackler Prize was awarded for his "seminal contributions to the field of natural product total synthesis through the syntheses of complex natural products by the use of new cascade reactions to rapidly achieve molecular complexity." The Shair research group focuses their efforts in two main areas: organic synthesis and chemical biology. Most projects involve syntheses of naturally occurring complex molecules that challenge the state-ofthe-art of organic synthesis. Target molecules are chosen that are structurally unique and have interesting, unstudied biological properties, enabling the Shair group to explore new areas of organic chemistry, particularly with respect to reactivity and selectivity. Of particular interest is the development of cascade reactions for each of the targets, in order to achieve the most efficient and rapid syntheses possible.



Phil Baran, Brian Stoltz and Matt Shair receive Sackler Prize at Tel Aviv University

ANDREW MYERS (PH.D. '95) began a new appointment in August 2009 as director of Pittsburgh State University's Kansas Polymer Research Center and Business and Technology Institute. In this role, Dr. Myers oversees the center and its research staff, scientists who perform groundbreaking research converting bio-based materials into plastics and foams. He also leads the staff at the Business & Technology Institute which focuses on small business support and economic development in the region. Prior to his current appointment, he worked as a primary investigator for TDA Research, where he developed a polymer and coatings nano-



composite research program by securing more than \$2.6 million in federal funding from organizations including the NSF, the Environmental Protection Agency, and NASA. During his ten years with TDA, he patented three inventions, published and presented numerous findings in nanotechnology, and was recognized as one of the EPA's Small Business Innovation Research "Success Stories." While at Rochester, Dr. Myers received his master's and doctoral degrees in chemistry under the direction of William Jones. He worked as a postdoctoral research associate at the University of Washington in Seattle, and served as a postdoctoral chemist for Union Carbide Corporation in Houston, Texas, where he devised and researched new catalysts for polypropylene.

RORY WATERMAN (B.S. '99) was

the recipient of a research award by the Alfred P. Sloan Foundation in 2009, one of the nation's most prestigious prizes for outstanding early career scientists. Since graduating from Rochester, Prof. Waterman has received his Ph.D. from the University of Chicago under the direction of Gregory L. Hillhouse (2004), conducted postdoctoral research in the laboratories



of T. Don Tilley at the University of California, Berkeley as a Miller Research Fellow, and in 2006, joined the Chemistry Department at the University of Vermont as an assistant professor. "The Sloan Research Fellowships support the work of exceptional young researchers early in their academic careers, and often at pivotal stages in their work," said Paul L. Joskow, president of the Sloan Foundation. Sloan Foundation awards are granted annually to select recipients in chemistry, physics, mathematics, computer science, economics, neuroscience, and evolutionary molecular biology. The unrestricted funds enable Sloan Fellows to pursue investigations of interest which further their research goals. Research in the Waterman Group focuses on problems in synthesis, catalysis, materials, and energy through the application of organometallic systems. These studies are directed at the discovery of new synthetic methods, the preparation of novel materials, and development of efficient or "green" syntheses through catalysis.

BRADLEY KRAFT (PH.D. '02) has received a tenure track assistant professorship in inorganic chemistry at St. John Fisher College in Rochester. In September 2009 he began teaching general chemistry there. While a graduate student at Rochester, he was a member of the Jones research group, where he worked on mechanistic investigations of carbon-fluorine bond activation by zirconium hydride complexes. Since graduation, he completed his postdoctoral research at Stanford, was married, and has worked at Ferro Corporation.



SUSAN SCHROEDER (PH.D. '02) an assistant professor of chemistry at the University of Oklahoma since 2006, was awarded an NSF CAREER Award, a grant from the National Science Foundation which supports the independent career development of young faculty. Prof. Schroeder's research program directs it efforts toward the long-term goal of RNA

structure prediction. The Schroeder lab explores the structure of encapsidated satellite tobacco mosaic virus (STMV) RNA, the structures and energetics of prohead RNA (pRNA), and the thermodynamic stabilities of noncanonical pairs at RNA helix ends. As genome sequencing projects produce increasingly vast amounts of data, the need for tools to interpret genomic sequence information at a structural level becomes increasingly urgent. The NSF funded research will provide fundamental knowledge to better understand the structure of encapsidated viral RNA, improve predictions of RNA structure from sequence, and thus elucidate dynamic viral RNA structure-function relationships. While at Rochester, Prof. Schroeder was a member of the Turner group.

JEREMY SMITH (POSTDOCTORAL FELLOW '03) now an associate professor at New Mexico State University, was awarded a Camille Dreyfus Teacher-Scholar Award in 2009. This award recognizes his research and teaching accomplishments as an independent faculty member. Research in the Smith lab involves the design and synthesis of transition metal complexes that are aimed at providing insight into important biological and industrial transformations. The Dreyfus Teacher-Scholar Award specifically recognizes his research on "nitrogen atom transfer" by three-fold symmetric iron nitrido complexes and the description of the electronic structures of thermally stable iron(IV) complexes. At Rochester Prof. Smith pursued his postdoctoral studies in the Holland group.

XIN WEN (PH.D. '05) has been awarded a Cottrell College Science Awards Single Investigator Award for her research entitled "Effects of Hofmeister Anions on Antifreeze Protein Activity" in 2009. Xin Wen is currently an assistant professor at California State University, Los Angeles. With this young investigator award, the Research Corporation supports the promise of the proposed research, as well as its potential for developing into a long-term research program, which will attract future support from other agencies. Prof. Wen's research interests are at the chemistry-biology interface; her group aims to understand the relationships between protein structure, dynamics, and function by integrating molecular biology techniques with biophysical methods (primarily NMR and CD).

WILLIAM DRELLES (B.S. '07) is now a member of the Peace Corps and is teaching chemistry at a high school in Cameroon, Africa.

FORMER FACULTY NEWS:

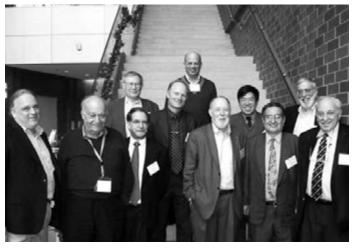
In 2008 **KEIJI MOROKUMA** was the recipient of the Imperial Prize and the Japan Academy Prize for his contributions in Theoretical Studies of Structure, Function and Reactivity of Molecules. The Imperial Prize is the highest academic award in Japan. Only one out of several Japan Academy Prize winners in all the sciences/engineering/



medicine is chosen to receive this award. The award ceremony took place on June 9, 2008 at the Japan Academy in Tokyo in the presence of the Emperor and Empress of Japan. Keiji Morokuma, joined Emory University in 1993 as the William Henry Emerson Chair of Chemistry and the director of the Cherry L. Emerson Center for Scientific Computation, where he is currently professor emeritus of theoretical chemistry. Before joining Emory, Prof. Morokuma was a faculty member at the University of Rochester from 1967-1977 and then worked for 16 years at the Institute of Molecular Science in Okazaki, Japan. The Imperial Prize was awarded in recognition of the integrated impact in chemistry of his work in understanding structure, function and reactivity of molecules by theoretical/computational approaches. Although up to nine people may receive the Japan Academy Prize each year, only two Imperial Prize awards are granted annually in the categories of humanities and natural sciences. The winners of the Imperial Prize were selected from among that year's recipients of the Japan Academy Prize, which includes a certificate, medal and prize of 1 million yen, which is the equivalent of about 10,000 dollars. Prof. Morokuma has received other honors including the International Academy of Quantum Molecular Science Award in 1978 and the Schrödinger Medal from the World Association of Theoretical Organic Chemists in 1993. He also served as president for the International Academy of Quantum Molecular Science in the early 2000's.

In December 2008, a symposium took place to celebrate the 60th birthday of **SHAUL MUKAMEL** honoring his seminal contributions to the field of ultrafast dynamics in the condensed phase and multi-pulse laser spectroscopy. Recent developments

and perspectives were presented at a two-day Symposium "Life in Liouville Space: 30 years of Theoretical Spectroscopy" at the University of California at Irvine (UCI). Prof. Mukamel, a faculty member in the Chemistry Department at the University of Rochester from 1982-2003, currently holds the position of Chancellor Professor of Chemistry at UC Irvine.



Shaul Mukamel and Distinguished Speakers at 60th Symposium

Among the symposium participants were leaders in the broad areas of Chemical Physics, Physical Chemistry, and Spectroscopy from all over the world. Noble Laureate, Rudy Marcus (Caltech), Bob Silbey (MIT), Yossi Klafter (TAU), Irvin Oppenheim (MIT), Graham Fleming (Berkeley), Sunney Xie (Harvard), Raoul Kopelman (Ann Arbor), Dwayne Miller (Toronto), also formerly on faculty at Rochester, and Paul Barbara (Austin) constitute an incomplete list of the invited speakers who were in attendance to celebrate Prof. Mukamel's birthday and honor his scientific contributions. Participants, many of whom are UR alumni, celebrated his long and productive career. Many of his former students and postdocs serve as faculty members at the universities all over the world and staff members at National Labs, including YIJING YAN (PH.D. '89) (Hong Kong), JASPER KNOESTER (POSTDOCTORAL FELLOW '90) (Groningen), VLADIMIR CHERNYAK, Senior Scientist, UR, 1992-2000 (Wayne State), ROGER LORING (POST-DOCTORAL FELLOW '88) (Cornell), LARRY FRIED (POSTDOCTORAL FELLOW '93) (Livermore), TORSTEN **MEIER (POSTDOCTORAL FELLOW '99)** (Marburg), YOSHITAKA TANIMURA (POSTDOCTORAL FELLOW '92) (Kyoto), FRANK SPANO (POSTDOCTORAL FEL-LOW '90) (Temple), ANDREI PIRYATINSKI (POSTDOC-TORAL FELLOW 2000) and SERGEI TRETIAK (PH.D. '99) (Los Alamos), among many others.

Prof. Mukamel is considered a founder of a new field of theoretical spectroscopy that addresses the goal of developing new spectroscopic techniques. Experimental Spectroscopy is an extremely precise measurement and characterization tool in a broad variety of materials ranging from biomolecules to organic and semiconductor (nano)structures. Theoretical spectroscopy, which provides unique interpretations of the measured signals in terms of the underlying physical phenomena, extends the capabilities of experimental spectroscopy from a precise experimental technique to a powerful tool for studying ultrafast dynamical phenomena. Prof. Mukamel's graduate level textbook "Principles of Nonlinear Optical Spectroscopy" has a wide reader audience, from graduate students to experienced researchers in the field of femtosecond spectroscopy. He is also the author of over 600 publications.

Mukamel family members also joined the Symposium: his wife Dana is Professor of Medicine at UC Irvine, and sons Eran and Ronen are graduates of Brighton High School in Rochester. Eran (B.A. Harvard, Ph.D Stanford) is currently a Postdoc at Harvard University, and Ronen (B.S. Harvard) is a current doctoral student in Mathematics at MIT.



Sergei Tretiak (Ph.D. '99), Andrei Piryatinski (Postdoctoral Fellow 2000), Misha Ovchinnikov, and Vladimir Chernyak

IN MEMORIAM:

KATHERINE E. FOSTER passed away in Rochester on May 29, 2009 at age 93. Kay Foster served as secretary to the Chair of Chemistry in the 70's and 80's. She was noted for her love of theater, having been a vaudeville dancer in her early years. She "retired" from the UR several times until, in her eighties, she retired for the last time. She is remembered by her family as having loved life, independence, travel, family and friends, and always being quick with a smile.

The Department of Chemistry also mourns the passing of:

- Ican D. Watkeys (B.S. '32, M.D. '36)
- Marvin L. Davis (B.S. '37, M.S. '39)
- C. Foster Aldridge (B.A. '40)
- Donald R. Koerner (B.S. '44, M.D. '46)
- Robert Schon Holdsworth (Ph.D. '47)
- Jack R. Kirchner (B.S. '54)

Feature Articles

In Memoriam Frank P. Buff (1924-2009)



Emeritus Professor of Chemistry, Frank P. Buff, passed away in Rochester on July 1, 2009 at the age of 85. He is survived by his wife of 52 years, Iva, and his two daughters and their families. Professor Buff was on faculty at the University of Rochester from 1950 until his retirement in 1994. He was a National Science Foundation senior postdoctoral fellow and a visiting professor at the Institute of Theoretical Physics in Utrecht, Netherlands from 1959-60.

Born in Munich, Germany on February 13, 1924, Frank Buff moved to San Francisco in 1937, where he graduated from Lowell High School in 1941. He received a Bachelor of Arts degree in Chemistry and Physics with highest honors from UC Berkeley in 1944. A World War II veteran, he served in the US Army in intelligence from 1944-1946. Following military service, he worked in 1946 as a Junior Chemist at Shell Development Company prior to continuing his doctoral and postdoctoral studies at the California Institute of Technology, working with the legendary John Gamble "Jack" Kirkwood. There he earned his Ph.D. in Chemistry in 1949, followed by a postdoctoral research fellowship awarded by the Atomic Energy Commission in 1949-50. During that period, he made two important contributions to the field of the statistical mechanics of liquids-the theory of solutions and the theory of liquid-gas interfaces-that occupied his interests throughout his professional career. In fact, both "Kirkwood-Buff" theories are still widely cited today.

By the time Prof. Buff arrived in Rochester in 1950, he was viewed as one of the "young men to watch" in the field of theoretical chemistry. At Rochester, Prof. Buff's courses and his mentoring were always viewed as intense and challenging, since few students could match his mathematical sophistication or meet his high standards. However, Ph.D. students JAMES E. SMITH (PH.D. '65), RONALD A. LOVETT (PH.D. '66), AND JAMES J. VIECIELI (PH.D. '70) were up to the task. He also influenced a number of undergraduates, including FRANK H. STILLINGER (B.S. '55) AND STEVEN SIBENER (B.S. '75). A long-time teacher of physical chemistry, Prof. Buff's knowledge of the private lives of famous scientists enlivened many of his lectures. Frank Stillinger of Princeton noted in an autobiographical piece published in the Journal of Physical Chemistry (J. Phys. Chem., 2004, 108, 19571-19573) that Professor Buff played an important role in shaping his life as a professional scientist; as a result of that influence he attended graduate school at Yale, working under the direction of Kirkwood, the same mentor who advised Buff at Caltech. Steven Sibener, now Carl William Eisendrath Professor of Chemistry at the University of Chicago, completed his undergraduate honors thesis with Prof. Buff in 1975.

Prof. Buff published numerous seminal papers in the fields of physical chemistry and physics, and in 1995, his work was included among the 1,000 most influential papers of the 20th Century as chosen by the American Physical Society and the American Institute of Physics in celebration of the 100th anniversary of the Physical Review and Physical Review Letters. He was a 60-year member of the American Chemical Society, and a member of Phi Beta Kappa, Sigma Xi, the American Institute of Chemists, the American Association for the Advancement of Science, and Fellow of the American Physical Society. During his long and distinguished academic career at the University of Rochester, Prof. Buff's research interests encompassed statistical mechanical theories of liquids, solutions, and interfaces, chemical kinetics, light scattering, critical phenomena, kinetics of nucleation, electrochemistry, physics of thin films, properties of zwitterions and capillarity. His research interests before his retirement were focused on the shape dependence of the grand potential and perturbative solutions of the Young-Laplace equation in external fields.

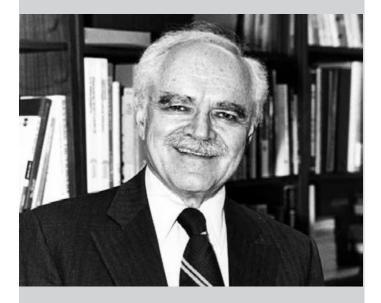
He is further remembered for important contributions to the Department including his participation, along with Professors Tarbell and Saunders in the 1960's, in the development of a long-range plan for the department. When the NSF announced the Center of Excellence Program, the Chemistry Department had the written proposal in hand to present to the administration. The long-range plan led, via the Center of Excellence award, to Hutchison Hall and a significant growth of the faculty in the late 60's and early 70's. In addition to his passion for science and 44-year long career as Professor of Chemistry at the University of Rochester, he enjoyed classical music, literature, photography, history, and art. He is lovingly remembered by his family as a devoted husband, father, and grandfather.

The Department of Chemistry conveyed condolences to the Buff family on behalf of all UR faculty, staff, and alumni. At Professor Buff's request there was no service and no formal mourning period. There was also no burial, as Frank Buff donated his body to the University of Rochester Medical School. The Buff family has requested that donations in Professor Buff's memory be made to the Visiting Nurse Service, 2180 Empire Boulevard, Webster, NY 14580, info@vnsnet.com. Chemistry alumni are also welcome to make donations to the Chemistry Alumni Research Fund in his memory.



View of Hutchison Hall from Goergen Hall

The Moses Passer Graduate Fellowship in Chemistry



In 2009, the Department of Chemistry was pleased and proud to announce the establishment of the Moses Passer Graduate Fellowship in Chemistry. The endowed fellowship fund was established by Mrs. Dorothy Rosenberg-Passer in January 2009 in memory of her husband, Dr. Moses Passer, who received his Bachelor of Science degree in Chemistry from the University of Rochester in 1945 and his Doctorate in Organic Chemistry from Cornell in 1948. After a distinguished career as Professor of Chemistry at the University of Minnesota Duluth, Dr. Passer became an executive at the American Chemical Society in Washington, DC, and served as Director of Education at the ACS for more than two decades. The Moses Passer Graduate Fellowship will be awarded annually by the Chemistry Graduate Studies Committee to a deserving doctoral student on the basis of his/her academic scholarship.

Through the generosity of Dorothy Rosenberg-Passer, the Moses Passer Graduate Fellowship in Chemistry is the latest in a series of fellowships offered to support meritorious graduate students. Other endowed graduate opportunities in the Chemistry Department include the DeRight, Weissberger, Lattimore, Sherman-Clark, and Ewart fellowships offered by the Chemistry Department and the Hooker, Messersmith and Sproull, Provost, and University Fellowships offered by the University of Rochester.

William D. Jones Receives an ACS Arthur C. Cope Scholar Award by Lois Gresh

The American Chemical Society (ACS) awarded an Arthur C. Cope Scholar Award to University of Rochester C. F. Houghton Professor of Chemistry **WILLIAM D. JONES** at its annual meeting in Washington DC in August 2009. One of the highest honors in Chemistry, the Cope Scholar Award was founded in 1984 and consists of \$5,000, as well as a \$40,000 unrestricted grant to support his research. Ten people receive the Cope Scholar Award each year.

Prof. Jones is one of the leading organometallic chemists of his generation, and as cited by the ACS, won the Award "for his fundamental studies of C-H and C-C bond activation, which have opened the door to exciting applications in synthesis and catalysis."

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 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 $Cp_2^2ZrH_2$ is capable of cleaving a wide variety of aliphatic C-F bonds, generating Cp_2^2ZrHF 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.

Prof. Jones won the ACS Award in Organometallic Chemistry in 2003 and has served as Associate Editor of the *Journal of the American Chemical Society* since 2003. He has published more than 163 professional articles and seven book chapters, and he has given more than 325 lectures and presentations at universities, meetings, and corporations. He earned his B.S. in Chemistry from MIT in 1975, and he earned his Ph.D. in Chemistry from the California Institute of Technology in 1979. He has been a faculty member of the University of Rochester since 1980.

Along with Prof. Jones, the other 2009 Cope Scholar Award Winners were Carlos F. Barbas III, Paul J. Chirik, Victor J. Hruby, Chaitan Khosla, Mohammad Movassaghi, Nicos A. Petasis, John A. Porco, Jr., David H. Sherman, and Erik J. Sorensen.

William D. Jones honored with the Edward Peck Curtis Award at Commencement, May 2009



2009 Edward Peck Curtis Award for Excellence in Undergraduate Teaching Awarded to William D. Jones

Professor William D. Jones was the recipient of the Edward Peck Curtis Award for Excellence in Undergraduate Teaching in 2009. Established in 1962, the 2009 award was conferred during the University Commencement ceremony at the Eastman Quadrangle on Sunday, May 17, 2009. The award annually honors University faculty members who have demonstrated extraordinary skill in the classroom and who have demonstrated a profound and lasting impact on their students. Beyond recognizing highly successful classroom performance, the award recognizes outstanding service in mentoring junior faculty and teaching assistants, as well as student advising.

Since joining the faculty at Rochester in 1980, William Jones, C. F. Houghton Professor of Chemistry, has taught numerous courses at both the undergraduate and graduate levels and served as Chairman of the Department of Chemistry from 2000-2003. He has also served for the past five years as Chair of the Department's Undergraduate Studies Committee with responsibilities for coordinating the department's undergraduate advising program. He has personally served as faculty advisor for more than 40 undergraduate students and for more than 45 undergraduate researchers, and has published twelve articles to date, resulting from the inclusion of undergraduates in his outstanding research program. Jones is noted for demonstrating brilliance and clarity in the classroom, having taught Freshman Chemistry (CHM 131/ CHM 132) for nearly a decade in the 90's, Advanced Lab Techniques (CHM 254) for five years and most recently, Honors Organic Chemistry Lab II (CHM 210). He is characterized by his students as a role model, an inspiration, and a friend.

Recognized for his groundbreaking work in organometallic chemistry, Jones research group focuses on the carbon-hydrogen bond in hydrocarbons and on exploring chemical ways in which that bond can be either broken or reformed to produce materials that are important for other products in addition to fuels. This University honor is the latest in a number of awards for Professor Jones: in 2009 he received an American Chemical Society's Arthur Cope Scholar Award (see related article) and in 2003, received the ACS Award in Organometallic Chemistry. Prior Peck Curtis awardees from the Department of Chemistry include Edwin Wiig (1963), Marshall Gates (1967), Jack Kampmeier (1974), James Farrar (1985), Joseph Dinnocenzo (2005), and Thomas Krugh (2008).

Richard Eisenberg elected to the American Academy of Arts and Sciences

Richard Eisenberg was elected to the American Academy of Arts & Sciences in April 2009 and was inducted into the Academy along with 208 other new fellows from 28 states and 11 countries at the Academy's headquarters in Cambridge MA, in the fall of 2009. Established in 1780 by the founding fathers of the nation, the Academy's elected members comprise leaders in all the academic disciplines, the arts, business, and public affairs. The Academy's unique strength lies in the distinguished leadership of its 4,000 Fellows and 600 Foreign Honorary Members and the wide range of expertise they bring to its multidisciplinary analyses of compelling contemporary issues. Current projects focus on science, technology, global security, social policy, the humanities, and education.

Prof. Eisenberg is honored by the Academy for his contributions to the fields of inorganic and organometallic chemistry, and as a researcher, teacher, leader, and mentor. He is considered a pioneer in the chemistry of platinum group element complexes for applications in solar energy conversion and homogeneous catalysis. His research focuses on light to chemical energy conversion in artificial photosynthesis and on the study of new catalysts for both organic and inorganic reactions. A distinctive attribute of Rich Eisenberg's chemistry research lies in 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 water into hydrogen using solar energy. An advocate for inorganic chemical education, he began teaching at Rochester in 1973, and also served as Chair of the Department from 1991 to 1994.

Prof. Eisenberg has been the recipient of numerous awards throughout his career, including early recognition through Sloan and Guggenheim Fellowships in the 1970's, and more recently, with the 2003 ACS Award for Distinguished Service in the Advancement of Inorganic Chemistry, the 2007 Morley Medal presented by the Cleveland ACS Section, and election as a Fellow of the American Association for the Advancement of Science in 2005. In 2009, he was elected into the inaugural class of Fellows of the American Chemical Society. Prof. Eisenberg currently serves as Editor-in-Chief of *Inorganic Chemistry*, the premier and most highly cited journal in its field, an editorship he has held since 2001. In 1996 he was named the Tracy H. Harris Professor of Chemistry by the University of Rochester.

Robert K. Boeckman, Jr. Receives the 2009 William H. Riker University Award for Excellence in Graduate Teaching

Robert K. Boeckman, Jr. was the 2009 recipient of the William H. Riker University Award for Excellence in Graduate Teaching, an award which annually recognizes a faculty member at UR who has excelled in graduate instruction, particularly in the University's doctoral programs. The award was presented at the 2009 Doctoral Graduation ceremony at the Eastman Theater on May 16, 2009. Bob Boeckman is the Marshall D. Gates Jr. Professor of Chemistry at the University, where he has served as chair of the Department of Chemistry since 2003.

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 Boeckman 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.

A graduate of Carnegie Institute of Technology (now Carnegie Mellon University), Prof. Boeckman earned his Ph.D. from Brandeis University in 1971. He was a professor at Wayne State University before joining Rochester's Chemistry Department. His academic honors include an Alfred P. Sloan Fellowship, a Research Career Development Award from the National Institutes of Health, and the Arthur C. Cope Scholar Award from the American Chemical Society. He also has been selected as a Fellow of the Japanese Society for the Promotion of Science and was awarded an Alexander Von Humboldt Stiftung Research Prize for Senior Scientists. In 2009 he was elected to the inaugural class of ACS Fellows. Since 1997, he has served as an associate editor of the *Journal of Organic Chemistry*.

As a teacher and mentor, Prof. Boeckman has trained dozens of successful chemists, most of whom are now working in industry and academia. As an advisor, he is renowned for being generous with his time and expertise and encouraging his students to set high professional standards for themselves. Since he began his career at Rochester his research group has consistently been among the largest research groups in the Department. Boeckman students have been rigorously trained and are recognized as having strong backgrounds in experimental approach and the ability to think creatively about ways to overcome the hurdles invariably encountered in complex and ambitious research undertakings. Prof. Boeckman has mentored more than 58 doctoral students and 48 postdoctoral fellows and is highly regarded for his forthright style, humor, dedication, and facility for nurturing and supporting his students professionally, postgraduation. He is also distinguished for his leadership and his commitment to strengthening the Department of Chemistry and the University.





Left: Robert K. Boeckman, Jr. and UR Trustee Edward Hajim at Riker Award Presentation 2009 Right: Richard Eisenberg and Robert K. Boeckman, Jr. at 2008 ceremony celebrating University Named Professors

Honorary Doctorate of Science Conferred upon Esther Conwell by SUNY Geneseo

Esther M. Conwell, Professor of Chemistry and Physics at the University of Rochester was selected to receive an Honorary Doctorate of Science degree from SUNY Geneseo on May 16th, 2009. This degree recognizes Prof. Conwell's many and varied remarkable careerlong contributions toward advancing scientific knowledge, and honors her leadership as a woman in science. Prof. Conwell is renowned for contributions to understanding electron and hole transport in semiconducting materials that helped to enable integrated circuits and organic electronic devices, both vital steps in the birth of the computer revolution. Prof. Conwell has also made important contributions to charge transport physics in DNA where hole motion along the helices is thought to be related to DNA photodamage. Her most recent work demonstrates that the transport is consistent with motion of delocalized polarons, accounting for many experimental observations on DNA.

Considered the preeminent woman pioneer of semiconductor device physics at the emergence of the electronics age, this latest tribute to her achievement was conferred by President Christopher Dahl and academic leaders at the afternoon SUNY Geneseo graduation ceremony. "Geneseo is proud to award an honorary doctorate to Prof. Conwell because of her extraordinary professional accomplishments and her longtime commitment to reducing barriers for women in science," said SUNY Geneseo President Christopher Dahl. "She is an exemplar of intellectual curiosity in and of itself and as a spur to invention." Although SUNY is the largest system of higher education in the U.S., very few honorary degrees are conferred. Honorary degree candidates are nominated by individual campuses, evaluated and recommended by a standing committee of distinguished faculty, and ultimately, approved by the full state-wide Board of Trustees.

This is just the latest in a series of lifetime achievement awards that demonstrate the esteem in which Esther Conwell is held in



Esther M. Conwell recognized by SUNY Geneseo with Honorary Doctorate of Science, May 2009

the scientific and educational community. She has been a member of the National Academy of Engineering since 1980, the National Academy of Sciences since 1990 and was elected to the American Academy of Arts and Sciences and the New York Academy of Sciences in 1992 and 1993, respectively. In 2002, Discover Magazine listed Prof. Conwell as one of the 50 most important women in the history of science for her significant role in understanding how electrons move through silicon and other semiconductors. In 1997, she became the first woman to receive the Thomas A. Edison medal, a major award from the Institute of Electronic and Electrical Engineers (IEEE). Most recently, she was awarded the Dreyfus Foundation's Senior Mentor Award (2005), the University of Rochester's Susan B. Anthony Award (2006), and in 2008, was recognized by the American Chemical Society with the ACS Award for Encouraging Women into Careers in the Chemical Sciences. This is the second Honorary Doctorate of Science conferred upon Prof. Conwell; in 1992, she received an honorary doctorate from Brooklyn College.



Statue Garden adjacent to Rush Rhees Library

Inaugural Magomedov-Shcherbinina Prize awarded to Sergey Kozmin

The Inaugural Magomedov-Shcherbinina Prize and Lectureship took place in Rochester on October 15, 2008. The first Prize was awarded to Sergey Kozmin, a rising star in the field of organic synthesis. Kozmin is Associate Professor of Chemistry at the University of Chicago and Centre Director of the NIH sponsored Chicago Tri-Institutional Centre

for Chemical Methods and Library Development. Prof. Kozmin was selected by faculty committee as a young chemist, (under the age of 40) who has demonstrated exceptional ability in research during the early years of his first independent academic appointment with the promise of outstanding accomplishments in the future. Kozmin is noted for his research program which aims to advance the chemistry and chemical biology of natural products in order to develop small-molecule libraries that rival the sophistication of naturally occurring secondary metabolites. This effort, which combines complementary expertise in organic synthesis, biochemistry, cell biology and animal pharmacology, enables the identification of an arsenal of new small-molecule agents and disease-related targets and pathways for basic and translational biomedical research.

The Magomedov-Shcherbinina Memorial Prize and Lectureship was created to memorialize Assistant Professor Nabi Magomedov, his wife Natalya Shcherbinina, and their three-year old son, Amir, who were killed on February 7, 2006 in a multi-vehicle accident. A memorial fund was established at the time of the tragedy by the Chemistry Department and Bausch & Lomb with the generous support of friends, family, alumni, and colleagues. Henceforth, the memorial Lectureship and Prize will take place annually. It was particularly moving and meaningful that Prof. Kozmin, the inaugural recipient of the Prize, was a friend and fellow countryman of the Magomedov family.

The inaugural event comprised an award ceremony presided over by Chair, Robert K. Boeckman, Jr. and Dr. Daniel Ammon of the Chemistry Department and Bausch & Lomb, respectively, followed by reminiscences of the Magomedov family by Prof. Boeckman, Dr. Ammon, Dagmara Magomedova and Prof. Kozmin himself. The Prize is an engraved medal fashioned in the likeness of the Magomedov family and an honorarium. Prof. Kozmin was also presented with a ceremonial Russian sword as a gift from the Magomedov family by Nabi's sister, Dagmara, who came from Russia to attend the event, representing the Magomedov extended family. Prof. Kozmin lectured on the "Practical Organic Synthesis to Unravel Chemical Biology of Complex Natural Products" to a packed audience of students, faculty and distinguished guests. One of the objectives of his group's research program is to elucidate the mechanism of action of complex natural products at the molecular level. Such compounds are discovered most frequently through phetotypic cell-based screening. Due to the significant progress in isolation and structure elucidation of new natural products, there is an increasing demand for efficiency in modern organic synthesis, which is required to provide practical access to rare and biosynthetically inaccessible secondary metabolites, in order to enable biological and pharmacological evaluation, en route to the ultimate development of new therapeutic agents. Prof. Kozmin discussed how the efficient chemical synthesis of complex natural products can enable identification of cellular targets of such compounds in several areas of cell biology, including cytokinesis, protein synthesis, and energy metabolism.

Following the custom for all distinguished lectureships in the Department, Prof. Kozmin had the opportunity to participate in individual meetings with colleagues throughout the day in Hutchison Hall. His lecture and award presentation were followed by a reception for the entire department and all guests. In a departure from a customary distinguished lectureship, the event was also attended by family, colleagues from Bausch & Lomb, non-scientists, and many friends who came from near and far to attend the Inaugural Prize presentation.

Sergey Kozmin received his Undergraduate Diploma at the Moscow State University in 1993. He obtained his Ph.D. in 1998 at the University of Chicago with Viresh H. Rawal, and completed postdoctoral studies at the University of Pennsylvania with Amos B. Smith, III in 2000. He began his independent academic career at the University of Chicago as an assistant professor; in 2006 he was promoted to the rank of associate professor. He has been recognized as an Alfred P. Sloan Fellow, an American Cancer

continued on next page 🖙

Robert K. Boeckman, Jr., Sergey Kozmin and Daniel Ammon (B&L) at award presentation, October 2008



Society Research Scholar, an Amgen Young Investigator, Glaxo-SmithKline Chemistry Research Scholar, a Camille Dreyfus Teacher-Scholar, and is a recipient of an NSF CAREER award.

In the summer of 2009 the award committee announced that Xiaowei Zhuang, Howard Hughes Medical Institute Investigator and Professor of Chemistry, Chemical Biology and Physics of Harvard University, has been selected as the second Magomedov-Shcherbinina Prize awardee. The next Magomedov-Shcherbinina Prize and Lectureship will take place in Rochester on April 7, 2010. All are invited to attend.



Symposium Highlights Frontiers in Nanomaterials Science for the 21st Century

NanoSymposium 2009, a two-day conference encompassing the overarching theme of the innovations in materials science and engineering that will be necessary to power, sustain, and heal the planet in the 21st century, took place on May 11-12, 2009 at the University of Rochester. The interactive program was organized and facilitated by Department of Chemistry Professors Todd D. Krauss and Lewis J. Rothberg, and featured a broad and diverse group of participants involved in nanomaterials science research relative to renewable energy and biomedicine. The conference was attended by over 180 faculty, undergraduate and graduate students from UR and nearby colleges, postdoctoral fellows, UR alumni, and local industrial associates from companies such as Kodak, Xerox, General Motors, Harris Beach, and Bausch & Lomb. The symposium took place in Goergen Hall, home of Biomedical Engineering and the Institute of Optics.

The Nanomaterials symposium was sponsored by the School of Engineering and Applied Sciences, the School of Arts and Sciences, and the School of Medicine and Dentistry and focused on significant research breakthroughs that are necessary in materials science and engineering to address the tremendous challenges facing humankind today - renewable energy, affordable healthcare, and a sustainable planet. UR is fortunate to have vigorous advocacy for these kinds of programs from Dean Robert Clark (SEAS) and Dean Stephen Dewhurst (URMC). Distinguished keynote speakers from around the world presented their latest discoveries, and the



program culminated in a joint poster session and conference reception where innovative materials science research at the University of Rochester, as well as in the greater Upstate New York region was discussed.

Prominent keynote speakers included Professors George Whitesides (Harvard), Louis Brus (Columbia University), Ashutosh Chilkoti (Duke University), Vicki Colvin (Rice University), and Michael Grunze (University of Heidelberg). Featured Rochester faculty members came from the Departments of Optics, Physics, Chemistry, Chemical Engineering, Electrical & Computer Engineering, Environmental Medicine, Dermatology, and Biomedical Engineering, who lectured on their most recent materials related research. Presentations included discussions of the new physics of single sheets of graphene, novel solar cell designs, nanoparticle based biological sensors, and the environmental impacts of nanomaterials.

As one of the country's top-tier research universities, the UR takes its scientific leadership role in the community very seriously. New startup companies in biomedicine and energy that will emerge in the coming years will naturally have a close relationship with the UR. The University seeks to support the continued entrepreneurial growth of nanomaterials research and development in the Rochester area and is committed to making available to the local community high quality scientific programs such as NanoSymposium 2009. In the Department of Chemistry, Professors Krauss and Rothberg were pleased to have the opportunity to assist in facilitating this symposium, showcasing the innovative research taking place within our institution and bringing distinguished outside speakers to Rochester. It is anticipated that the symposium will be the first in a series of initiatives that will lay the groundwork for a vibrant interdisciplinary materials science program encompassing many faculty at Rochester, as well as collaborative efforts with local industrial scientists interested in the emerging field of nanomaterials science.

Symposium Participant Vladimir Dyakonov with Speaker Ching Tang, NanoSymposium, May 2009

The 2009 Biological Chemistry Cluster Retreat by Doug Turner

The Biological Chemistry Cluster was founded six years ago at the suggestion of Robert K. Boeck-

Man, Jr. The Cluster now consists of eleven groups from the Department of Chemistry and five groups from the Department of Biochemistry and Biophysics. Two goals of the Cluster are to increase interactions between groups doing Biological Chemistry at the University of Rochester and to increase appreciation of Biological Chemistry research. The main medium for achieving these goals is an annual Retreat. The fifth annual Retreat was held on June 3-4, 2009. It was funded by Provost Ralph Kuncl as a function of the University Committee for Interdisciplinary Studies (UCIS), which also funded all but the first Retreat. Prof. David McCamant 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 3rd with two talks to a packed audience in Hutchison Hall 473. The first talk was on "Spectroscopic Approaches to Protein Aggregation Diseases" by Sean Decatur, Professor of Chemistry and Dean of Oberlin College. His work was subsequently highlighted in the cover story, "Tools for Amyloids," in the June 15th issue of *Chemical & Engineering News*. The second talk was on "Molecular Simulations of Ribozyme Catalysis" by Darrin York, Associate Professor of Chemistry at the University of Minnesota. This continued a tradition of having one speaker from the protein community and one from the nucleic acid community. Both speakers enjoyed visiting Rochester in the absence of snow.

The Retreat reconvened in the Staybridge Suites at 9 AM the next day with 80 attendees. The previous three Retreats were held at the Glen Iris Inn in Letchworth State Park. The Staybridge Suites

R. Fasan, K. Bren, D. Goldfarb, L. Vacca Michel (Ph.D. '06), D. Turner, D. York, D. McCamant, J. Wedekind, N. Shankar (Ph.D. '08), D. Krysan, B. Nilsson, and the Genesee River, Biochemistry Cluster Retreat 2009



hotel opened last year across the Genesee River from the University and next to the footbridge. The University is attempting to build up the 19th Ward area and the BC Cluster decided to help by introducing many people to the hotel. The speakers who stayed at the hotel spoke highly of the accommodations and particularly enjoyed the view of the University right across the Genesee River.

The day started with a continental breakfast and session of 16 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 NEEL SHANKAR (PH.D. '08) from the Nixon Peabody law firm, LEA VACCA MICHEL (PH.D. '06) currently working at Johnson and Johnson as an employee of Kelly Contractors but about to start as an Assistant Professor at the Rochester Institute of Technology, Damian Krysan an Assistant Professor in the Pediatrics Department, and Darrin York. Neel said that a Career Panel discussion at a previous retreat led him to consider a career in patent law. A common theme of the discussion was that careers rarely go in a direct line. For example, Damian Krysan started with a Ph.D. in organic chemistry from Northwestern and a postdoc with **LANNY LIEBESKIND (PH.D.** '76) now at Emory, followed by a job in the pharmaceutical industry before getting an M.D. degree at the University of Michigan. In contrast, Darrin York started Medical School at the University of North Carolina and quickly transferred into their Ph.D. program in Chemistry so that he could do research in computational chemistry. The discussants gave interesting, candid answers to questions and inspired the audience to think about their own career plans. This was facilitated by the buffet lunch that followed, where participants enjoyed informal interaction.

The afternoon program included five scientific talks from members of UR labs. Charlie Bowerman from the Nilsson group talked about "Aromatic and Hydrophobic Interactions in Peptide Self-Assembly;" Damian Krysan about "Chemical Genetics for the Discovery and Mechanistic Study of Antifungal Small Molecules;" Clara Kielkopf from the Biochemistry and Biophysics Department on her lab's work on RNA splicing; Dave Goldfarb from Biology on his lab's "Screening Large Chemical Libraries for Small Molecules that Affect Age-Related Diseases," and **ILYAS YILDIRIM (PH.D. '09)** from the Turner group on free energy computations for tandem GA pairs in RNA.

Much information was exchanged throughout the two days and new connections were made that can enhance Biological Chemistry at UR. Several attendees were undergraduates participating in the Department's summer Research Experience for Undergraduates program, which Tom Krugh directs. The Retreat gave all participants a broad overview of Biological Chemistry.

John Huizenga Research Memoir Published by the University of Rochester Meliora Press

The Chemistry Department is pleased to announce that John Huizenga's research memoir entitled "Five Decades of Research in Nuclear Science" is expected to be published by the Meliora Press in 2009. Throughout his 50-year scientific career, John Huizenga has been a towering figure guiding research at the frontiers of science, having made exceptional contributions to nuclear science and technology. His legacy continues in the impressive body of knowledge and insights recorded in his many scientific articles and books and lives on in his students, whose intellectual formation and scientific careers he so markedly influenced. A history of his research career is now described in detail in this volume. The book summarizes Prof. Huizenga's research in the field of nuclear science carried out at the Argonne National Laboratory and the University of Rochester during the last half of the twentieth century. Also included are descriptions of selected travels, government service, and other activities related to his professional career.

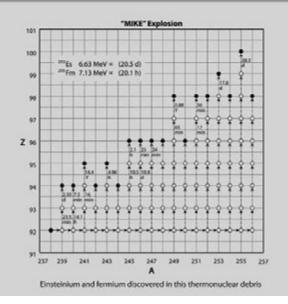
During his initial years at Argonne National Laboratory, Prof. Huizenga participated in a research program to irradiate ²³⁹Pu in high-flux-neutron reactors for long periods of time to produce transplutonium nuclei, including possible new elements. This then largely unexplored region of the periodic table was rightly predicted to be a rich and fertile source of new chemical and nuclear information. The production and study of these new highly-deformed actinide nuclei were of basic scientific interest, making possible more extended studies of such fields as nuclear structure, nuclear systematics, nuclear fission and heavy-element chemistry. Additionally, very long irradiations of ²³⁹Pu opened up the possibility of making sufficient amounts of transplutonium nuclei to be used as targets in subsequent accelerator experiments, enabling the probe of their excited-state structures.

On November 1, 1952 the first thermonuclear device (named "Mike") was tested on an island in the South Pacific. Recognizing the possibility that debris from "Mike" would contain new elements, early analyses of elemental plutonium and curium samples demonstrated that high-mass isotopes of these elements had been created, confirming that "Mike" produced a gigantic instantaneous number of neutrons. These titillating results spread like wildfire from the Atomic Energy Commission's office in Washington, DC to scientists in national laboratories across the nation. The race for the discovery of new elements was under way! Eventually, scientists from three national laboratories collaborated in a joint publication announcing the discovery of the new elements einsteinium and fermium.

After a Fulbright Fellowship sabbatical leave in Amsterdam, Prof. Huizenga initiated a study of the abundance of selected

JOHN R. HUIZENGA

FIVE DECADES OF RESEARCH IN NUCLEAR SCIENCE



elements in meteorites, especially chondrites, a class of stony meteorites thought to give a good representation of the cosmic element abundances. His interest in this subject was piqued by the observation that the two very different neutron capture processes, studied in the laboratory each had a very similar astrophysical counterpart. Supernovae explosions, like the "Mike" explosion, release gigantic numbers of neutrons for a small fraction of a second. While red giant stars, like reactors, produce a steady flux of neutrons for long periods of time. Each of these processes produces a unique fingerprint of heavy element abundances.

Initially introduced to nuclear fission in early 1944 on the Manhattan Project, Prof. Huzienga worked for years to better understand this extremely complex, but fascinating, nuclear reaction. A variety of experiments were designed to examine the intermediate transition-state nucleus, the highly deformed saddle-point configuration through which the nucleus passes on the way to fission. Studies of the mass, energy and angular distributions of the fission fragments were made for a wide range of targets, projectiles and energies. On another front, major progress was made in understanding the way excited compound nuclei de-excite, with emphasis on the decay competition between fission and other open-exit channels for actinide nuclei. To interpret these experiments, extensive experimental and theoretical studies were conducted of the dependence of the nuclear level density on excitation energy, angular momentum, isospin, nuclear shells, and nuclear deformation. Investigations of nuclear fission culminated in the popular reference book entitled "Nuclear Fission," which Prof. Huizenga co-authored with R. Vandenbosch.

In 1967, Prof. Huizenga joined the faculty at the University of Rochester as Professor of Chemistry and Physics, eventually serving as Chair of the Department from 1983-1988. The University's Nuclear Structure Research Laboratory had just acquired a state-of-the-art Emperor tandem van de Graaff. He immediately took advantage of the availability of high resolution beams of energetic helium ions by embarking on a systematic study of the single-particle and collective excited states of actinide nuclei by reaction spectroscopy. Direct reaction studies produced a large amount of new data on the spins and energies of neutron, proton and collective states of highly-deformed actinide nuclei and contributed to the rapid development of theoretical models of such nuclei.

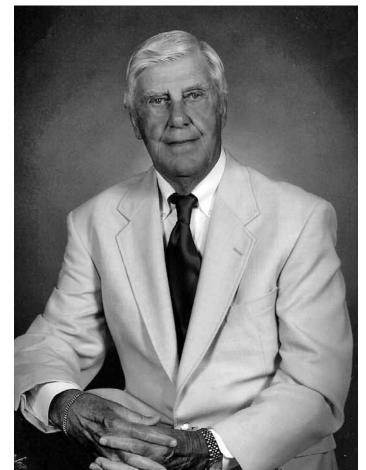
The decay modes of actinide muonic atoms were investigated at the Los Alamos Meson Physics Facility (LAMPF). The experiments, designed to determine the muon capture rates in neutron rich, actinide nuclei, measured the time difference between the arrival of a muon in the target and the appearance of any reaction product associated with the capture of the muon by the nucleus. Of particular interest was the prompt fission resulting from internal conversion, where the transition energy between inner shells of the muonic atom is transferred directly to the nucleus. A third major research program carried out at Rochester was a study of heavy-ion-induced reactions. A new type of reaction mechanism was discovered, which became known as strongly damped or deep inelastic collisions. Detailed studies were made of the energy dissipation, the nucleon transfer, and the microscopic time scale associated with these collisions. This new process yields two fragments in the exit channel, each with a Gaussian Z (atomic number) distribution centered near the Z values of the projectile and target. The variances in the Z distributions are strongly correlated with the magnitude of the energy dissipation. Large amounts of radial kinetic energy are dissipated in these reactions, resulting in kinetic energies of the fragments in the exit channel being as small as the Coulomb repulsive energy of two touching highly deformed fragments.

The experimental relations between charge (Z), mass (A), and energy loss of the fragments were analyzed in terms of an independent-particle transport model. In this model, transport of mass, charge, energy, linear and angular momentum in a strongly damped collision is attributed to the stochastic exchange of individual nucleons between reaction partners. Quantitative agreement between experiment and theory was obtained, including the energy-loss dependence of isobaric and isotopic fragment distributions, when account is taken of the Pauli exclusion principle. In collaboration with Prof. W. Udo Schröder, a 685-page article entitled "Damped Nuclear Reactions" was published by Plenum Press.

After a long and illustrious career, John Huizenga retired from the University of Rochester in 1991 and now resides in Pinehurst, North Carolina. Among his professional awards are a Fulbright Fellowship (1954-55), two Guggenheim Fellowships (1964-65 and 1973-74), the Department of Energy's E. O. Lawrence Memorial Award (1966), the American Chemical Society's Glenn T. Seaborg Award (1975), Calvin College's Distinguished Alumni Award (1975) and the Leroy Randle Grumman Medal for Outstanding Scientific Achievement (1991). Prof. Huizenga is a member of the National Academy of Sciences and the American Chemical Society, and a Fellow of the American Academy of Arts and Sciences, the American Physical Society and the American Association for the Advancement of Science.

Those alumni wishing to obtain a copy of "Five Decades of Research in Nuclear Science" are invited to contact the Department of Chemistry. Please contact Debra Haring, haring@ chem.rochester.edu or 585-275-2915 with your request.

John R. Huizenga, Tracy H. Harris Professor Emeritus of Chemistry



Student Awards and Accolades

Last year set the record for student recognition and honors in the Department of Chemistry! See also Commencement Awards on page 58.

BRIAN PALMISANO (B.A. '09) was the first undergraduate student at the University of Rochester to receive an Undergraduate Scholarship from the National Institutes of Health. A graduate of the Class of 2009 who majored in Biochemistry and Chemistry, Brian was selected from a pool of nearly 250 undergraduate scholars nationwide who are pursuing science, social-science, and health-related majors. The NIH Scholarship awards up to \$20,000 in scholarship funds for college, a 10week paid summer research laboratory experience at an NIH facility after graduation, formal seminars and professional mentoring, and a full-time paid NIH research position following completion of the awardee's doctoral degree. During his senior year, Brian worked with Dr. Janet Sparks in the Department of Pathology on insulin signaling in a rat cell model.



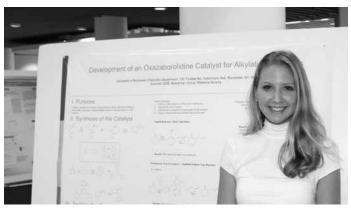
Each spring, the Rochester Center for Community Leadership recognizes undergraduate students and organizations that have made significant contributions to campus life. Nominated by faculty, staff, and peers, Student Life Award recipients represent diverse interests, talents, and accomplishments. In 2009, Chemistry undergraduate, **PAUL ALPERIN** was awarded the Eli & Mildred Sokol Prize as a sopho-

more who has emerged as a leader expected to contribute sig-

nificantly to the welfare of his fellow students in the next two years. Take 5 Scholar **DANIEL NASSAU (B.A. '09)** was awarded the Seth H. & Harriet S. Terry Prize in 2008, an award given to a male member of the senior class who, by his industry, character and honorable conduct, has done the most for the life and character of the undergraduate community.

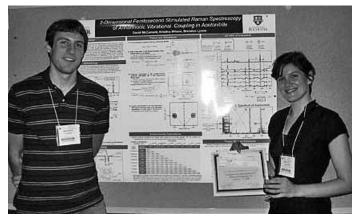


VISHAL ANUGU (B.A. '09) received an Intramural Research Training Award (IRTA) Fellowship from the NIH for 2009-2010. The Postbaccalaureate IRTA program provides opportunities for recent college graduates to spend a year engaged in biomedical research at the NIH. Under the direction of Professor Harry Stern, Vishal worked on a protonation state correction for protein-ligand binding. With this fellowship, he plans to study methods for improving imaging in Diagnostic Radiology before pursuing a medical degree.



Rebecca Murphy (B.S. '09) at REU Poster Session 2008

REBECCA MURPHY (B.S. '09) was selected to present her senior chemistry research project at the Merck Index Women in Chemistry Poster Session at the 238th ACS National Meeting in Washington DC. The Merck awards are presented at the Women in Industry Breakfast, in conjunction with a symposium sponsored by the Women Chemists Committee. Participating in this program provides invaluable experience for young women scientists to attend a national meeting, present their work, and to interact with women role models from both industrial and academic settings. Rebecca was a member of the Boeckman group while at Rochester and is currently a graduate student at UC Berkeley.



Brendon Lyons and Kristina Wilson with award-winning poster

Chemistry third-year graduate student, **KRISTINA WILSON** along with 5th-year Masters student **BRENDON LYONS (B.S. '08)**, received the Physical Chemistry Student Poster Award at the Fall 2008 ACS meeting in Philadelphia, PA. Both students are members of the McCamant research group. Their poster, which was one of six that were selected for this award, was entitled "2-Dimensional Femtosecond Stimulated Raman Spectroscopy of Anharmonic Vibrational Coupling in Acetonitrile."



MEAGAN EVANS, a third-year graduate student in the Jones Group, received the Best Presentation award at Brock University's 41st Annual Inorganic Discussion Weekend which took place in November 2008 in St. Catharines, Canada. Meagan was recognized for her work on C-H bond activation of fluorinated aromatic hydrocarbons by [Tp`Rh(CN-neopentyl)] which is

used to determine the stability of the $Rh-C_{aryl}$ bond and proves to be strongly dependent on the number of ortho fluorines.

Two graduate students **SARAH BOWMAN** (Bren Research group) and **CHRISTOPHER EVANS** (Krauss Research group) from the Department of Chemistry were selected to represent the U.S. delegation of students supported by NIH and NSF, respectively, and attended the 59th meeting of Nobel Laureates in Lindau Germany in July 2009. The Lindau Nobel Laureate Meetings provide a globally recognized forum for the exchange of scientific knowledge between Nobel Laureates and young researchers - the 59th Lindau meeting focused on the discipline of chemistry. Sarah and Chris join a select group of graduate students from Chemistry who have been offered this privilege in the recent past; Amy Ensign and Lisa Carlson were awarded this opportunity in 2007, and Chemistry alumnus, JEFF PETERSON (PH.D. '07) was selected to attend the Lindau meeting in 2005.

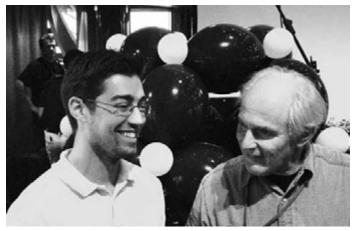


Sarah Bowman and Richard R. Ernst, winner of the Nobel Prize in Chemistry in 1991

JESSICA SMITH, a first year-graduate student in the Fasan 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. The award is based on Jessica's academic record and her research proposal submitted to the National Science Foundation last fall entitled "KFE8 Peptide Self-Assembly Directed by Oligonucleotide Recognition Events." **DANIEL EVERSON**, a first year graduate student in the Weix group was awarded an honorable mention from the NSF Graduate Research Fellowship program for his research proposal application "The Direct Reductive Coupling of Two Organohalides." The Weix group does research on new reactivity, the design of new multimeric catalysts, and the development of these ideas into useful synthetic methods.



Chris Evans with Sir Harold Kroto who shared the 1996 Nobel Prize in Chemistry for the discovery of fullerenes



CHRISTOPHER EVANS was selected to receive a 2009 SPIE Scholarship in Optical Science and Engineering. This meritbased scholarship is intended to enhance students' educational and professional development as they pursue their educational and career goals in optics and photonics. Chris was honored by the International Society for Optical Engineering along with other scholarship recipients at the SPIE Optics and Photonics Conference which took place in San Diego, California in August 2009.

Researchers determined the structure of a key genetic mechanism at work in bacteria, including some that are deadly to humans, in an important step toward the design of a new class of antibiotics, according to an accelerated publication that appeared online on April 17, 2009 as a "paper of the week" in the *Journal of Biological Chemistry (J. Biol. Chem.*, **2009**, *284*, 11012-11016). Along with Professor Joseph Wedekind, senior technician Jolanta Krucinska and collaborator, Vahe Bandarian (Univ. Arizona, Tucson) the work was performed in the Department of Biochemistry & Biophysics at URMC by doctoral students **ROBERT C. SPITALE (PH.D. '09)** and Andrew T. Torelli, who played key roles in the structure determination and refinement. The work was funded in part by research grants from the National Institutes of Health and the National Institute of General Medical Sciences. The article represents one part of the thesis research of Rob Spitale, who defended his doctoral thesis in Chemistry in April and earned his Ph.D. in May 2009 under the direction of Professor Wedekind, a member of the Biological Chemistry Cluster.



Pingwu Du (Ph.D. '09) with his wife Jingxue Chen and son Alexander at Commencement 2009

PINGWU DU (PH.D. '09), a fifth-year graduate student in the Eisenberg Group, was selected as a recipient of the 2009 Young Investigators Award. Pingwu presented his research at the 2009 Young Investigator Symposium of the Division of Inorganic Chemistry of the American Chemical Society at the National ACS meeting in Washington DC in August 2009. The DIC symposium honors talented young inorganic chemists, and provides a high-profile forum for them to present their research results.

WESLEY ASHER, a second-year graduate student received the 2009 Edward Peck Curtis Award for Excellence in Teaching by a Graduate Student. This award recognizes his outstanding performance as a teaching assistant in a wide variety of chemistry courses, his dedication and commitment to students, and his exceptional service to the Department of Chemistry. The award was conferred at a special luncheon with Provost Kuncl and Vice-Provost Jacobs in May 2009. In the Department of Chemistry, Wesley joins graduate students Mary Lenczewski, Amy Ensign, Lisa Carlson, and Jerry Manbeck, all of whom were recognized with this award in the recent past. Wesley is a member of both the Krauss and Bren groups.

KAREN CHIANG, a third-year graduate student in the Holland lab, received travel awards from the UR Graduate Women in Science (GWIS) and Eli Lilly/ACS Women Chemists Committee (WCC) to attend a scientific meeting in 2009. The mission of GWIS is to provide mentoring and support for the professional and personal development of all graduate women at the University of Rochester



Medical Center and College of Arts and Sciences. The ACS Women Chemists Committee (WCC) and Eli Lilly and Company sponsor their travel award programs to provide funding for undergraduate, graduate, and postdoctoral female chemists to travel to meetings to present the results of their research, in an effort to increase the participation of women in the chemical sciences. Karen received the awards based on her leadership potential and her research on binding to three-coordinate iron complexes, which was recently published in *Inorganic Chemistry*.

MATTHEW LIPTAK, a postdoctoral fellow in the Bren lab, was awarded a 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 for three years of postdoctoral study. 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.

The Bren Research Group 2009 Mehmet Can, Kara Bren, Sarah Bowman, Andrea Lee, Erin Knappen, Eric DeCoste, Amy Ensign, Matthew Liptak, Jesse Kleingardner, Wesley Asher

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Robert K. Boeckman, Jr.

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



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 2008-2009 academic year, **ROBERT K. BOECKMAN, JR.** completed his sixth year as the Chair of the Chemistry Department. Professor Boeckman will continue as Chair for a new 3-year term starting in 2009-2010. 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 is undergoing refinement and application 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. 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 a oxidation of aldehydes and other applications. Work on the synthesis of novel intercalator/metal chelator systems and novel bis-N-oxides as novel antitumor diagnostic/therapeutic molecules is also continuing.

VENKAT SRINIVASAN (PH.D. '09) defended his thesis in December 2008, and moved to Scripps La Jolla, where he began work as a postdoctoral associate in Dale Boger's group. **XINYI SONG (PH.D. '07)** is in his third year as a postdoctoral fellow at Scripps in Florida working under Ted Kameneka and Bill Roush, and KE CHEN (PH.D. '07) completed her postdoctoral work with Phil Baran at Scripps in La Jolla and has taken a position with Bristol-Myers Squibb in their process chemistry group, where she joins her spouse SAM ZHANG (M.S. '04). Other recent graduates of the group, DAVID MIN (M.S. '06) and PHILIP WARBURTON (M.S. '06) are pursuing employment as chemists in industry. Nate Genung, Yan Zhang, and John Miller continue their research in the group. Matt Betush delivered his 3rd year seminar and continues working on a nanochemistry collaboration with industry. George Arab and Bryan Ohman completed their 2nd year oral exams in July and are working on total synthesis projects 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. UR undergraduates **REBECCA MURPHY (B.S. '09)** and **JOHN BERTOLA (B.A. '09)** worked with the group during the year, as well as during the prior summer as REU participants, with Rebecca completing her B.S. senior thesis. Rebecca began her Ph.D. studies in Chemistry at UC Berkeley in the fall and John is pursuing a Masters in Education at the UR Warner School, having received a Noyce scholarship, and plans to teach chemistry at the high school level. In the summer '09, three undergraduates worked in the group as part of the NSF REU program: Doug Tusch is from RIT, where he works with Boeckman group alumnus JEREMY CODY (PH.D. '04), Toby Maxwell from SUNY Geneseo, and David Kaphan, a freshman at UR. Dave and another rising sophomore, Emily Hart, will work in the group during the 2009-2010 academic year.

Finally, Professor Boeckman was honored to receive the 2009 William H. Riker University Award for Excellence in Graduate Teaching and thanks all of the Boeckman current and former students who participated in the Riker award nomination for their support. 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 biomolecules.

CONTACT

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The **KARA BREN** group welcomed four new members in the past year. Two are the group's first postdocs, Matthew Liptak and Andrea Lee. The group recently celebrated the awarding of an NIH Postdoctoral Fellowship to Matt who is studying the effect of heme conformation on electronic structure. The group is benefiting from Matt's expertise in computational chemistry, resonance Raman, and EPR spectroscopy. Andrea, in a joint project with Todd Krauss, has experience with heme protein folding and single-molecule biology, and is investigating cytochrome c folding on the single-molecule level. In addition to the two postdocs, Erin Knappen officially joined the group as a first-year graduate student after having already completed two successful summers of research. Erin is continuing her studies of a low-potential di-heme cytochrome. In addition, FERDOUS ZANNAT (B.S. '09) joined the lab to study the relationship between relaxation properties and axial ligand strength in cytochromes.

The veteran members of the Bren group are continuing with their investigations of heme protein biophysical and bioinorganic chemistry. Amy Ensign is completing her thesis work on fluorescence studies of cytochrome c folding, and recently has been investigating the effects of protein immobilization on folding. Wes Asher also is on the Bren and Krauss group's folding project and has developed the use of heme tagging to introduce a chromophore for studying folding. Other Bren group graduate students are continuing the group's long-term project on spectroscopic studies of cytochromes c, with an emphasis of application of NMR to study

Kara Bren serving as a marshall at the 2009 doctoral graduation



electronic structure and dynamics: Sarah Bowman is developing NMR methods for probing heme-ligand interaction, Mehmet Can is probing the effect of the heme pocket on heme axial ligand dynamics, Eric DeCoste is working with the model system microperoxidase and other heme peptides, and Jesse Kleingardner is studying heme conformation in mitochondrial cytochromes *c* and metal-substituted cytochromes *c*.

In addition to the range of methods already employed by the Bren lab, Kara and Sarah performed the lab's first experiments at a synchrotron. In collaboration with Nicholai Lehnert (University) of Michigan) and Serena DeBeer George (Stanford University), they visited the Advanced Photon Source at Argonne National Laboratory to collect Nuclear Resonance Vibrational Spectroscopy (NRVS) data. This approach promises to provide details on vibrations involving the iron that can not be seen using other methods. Kara also commenced a collaboration with Prof. Joseph Wedekind (URMC, Biochemistry and Biophysics) on X-ray crystallography. Ongoing collaborations in which the Bren group is involved are with Kristoffer Andersson (University of Oslo) on EPR, Marcel Swart (University of Girona, Spain) on computational studies, Sean Elliott (Boston University) on 2D-IR.

Bren group alumni had much exciting news to report. XIN WEN (PH.D. '04) was awarded a Cottrell College Science Award for her studies of antifreeze proteins at California State University, Los Angeles. RORY (MELENKIVITZ) WATERMAN (B.S. '99), Assistant Professor at the University of Vermont, was named a Cottrell Scholar and additionally received a Sloan Fellowship for his work on catalytic bond formation. LEA VACCA MICHEL (PH.D. '06) accepted a position as an assistant professor of chemistry at RIT.

Along with Lea Vacca Michel, Kara was on the organizing committee for the successful 10th Annual Upstate NY NMR Conference held in Rochester in October, 2008. In the past year, Kara accepted a position on the Editorial Board of *Inorganic Chemistry*, and was named Chair-Elect of the Bioinorganic Subdivision of the American Chemical Society.

Esther M. Conwell

Research Professor



RESEARCH INTERESTS

Transport along the base stack in DNA. Optical properties of DNA, particularly those associated with excitons. Electrical and optical properties of organic semiconductors, particularly conjugated polymers.

CONTACT conwell@chem.rochester.edu

Some years ago ESTHER CONWELL and her postdoc, Denis Basko predicted that solvation of an electron or hole added to the base stack of DNA would result in the electron or hole becoming a polaron spread over several sites (bases). Our calculations showed that the polarization of the water in this process results in the energy of the excess electron or hole being decreased by ~ 0.5 eV. Over the years there have been some experiments that are best explained by a hole added to the base stack becoming a polaron spread over a few sites, but, according to the literature, there are still many who believe that the holes are confined to a single base. This past year two experiments were published by the group at Northwestern, including FRED LEWIS (PH.D. '68), that point more directly to the holes forming polarons spread over 3-4 sites, in agreement with our original prediction. The Conwell group is now doing further calculations based on the conditions set up in the recent experiments to show they are satisfied by the polarons we predicted.

As has been noted earlier, thermal fluctuations in DNA are quite large and have been shown to affect base orientations and energies considerably. Our calculations that predicted the polarons did not take the fluctuations into account. It has been suggested that the fluctuations could result in localizing the polaron to one site. The results of the experiments mentioned above make this quite unlikely. However, the experiments must measure a time average of the polaron properties and it is reasonable that the fluctuations might cause the wavefunction to vary in an erratic way with time. We have set up the calculations, using the program cp2k, to determine the variation of the wavefunctions on a fs time scale. The calculations use molecular dynamics to introduce the thermal motions of the atoms and quantum mechanics to determine the resulting wavefunctions and energies. From the short-time variation of the position of the wavefunction we should be able to determine the diffusion rate of the polarons, which has not yet been measured.

Goergen Hall, Computer Studies Building, Carlson Library, Hutchison Hall, and Hylan Hall (left to right)



Joseph P. Dinnocenzo

Professor of Chemistry



RESEARCH INTERESTS

Chemistry of organic ion radicals; mechanistic and physical organic chemistry; design and testing of new photoresponsive polymeric materials.

CONTACT jpd@chem.rochester.edu

JOE DINNOCENZO and his group continue to pursue a variety of problems in photoinduced electron transfer and related chemistry. In one project we described our most recent research on a new kind of reactive intermediate in photochemical reactions that we call a "bonded exciplex". Bonded exciplexes have many of the same properties as conventional exciplexes except that they contain a strong bond between the electron donor and electron acceptor partners of the exciplex. Over the past year we initiated a collaboration with Prof. Björn Roos (University of Lund) - an expert in excited state calculations - to gain further insight into the electronic character of bonded exciplexes. In other work, we reported several rigid polymeric materials that are capable of upconversion from green to blue and from blue to UV; the latter being a first in such materials. Most recently, we applied several transient laser methods to determine accurate oxidations for a variety of aromatic compounds, including benzene and toluene, which have been sought after for decades. Finally, the group continues to delve

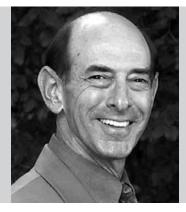


into the mechanistic subtleties of how organosilane cation radicals react with nucleophiles. Joe presented several talks on the group's research at colleges and universities over the past year, including the Lise Meitner-Minerva Center Symposium at the Hebrew University in Jerusalem.

On the teaching front, Joe began two new courses this past academic year. In the fall he began teaching CHM 433 (Physical Organic I) after a sixteen year hiatus. Joe looks forward to teaching the class again this fall and to introducing some changes based on the experiences last year. In the spring Joe taught CHM 210 (Honors Organic Laboratory II) - a course he had not taught in over 20 years! Joe was blessed with a wonderful group of students in CHM 210, who were eager participants in an experiment to introduce Peer Led Teaming Learning (aka Workshops) into the course. Joe was ably assisted in this endeavor by Ms. Terrell Samoriski, who helped with the implementation and evaluation of the workshop model. The workshops were a great success in CHM 210 and Joe will be working with a number of other faculty over the next three months to incorporate the workshops in labs model into a grant proposal to the Howard Hughes Medical Institute to, among other things, refine and expand the model within the University and, hopefully, beyond.

As for group news, Mary Lenczewski is close to wrapping up her Ph.D. research on the stereochemistry of organosilane cation radical substitutions. Third-year graduate student Pu Luo is making good progress on using stereochemical probes to test the reversibility of $S_N 2$ reactions on organosilane cation radicals and on discovering a novel route to generate silane cation radicals. David Turner, a second-year student is working on understanding the mechanism(s) of organo-germane and stannane cation radical fragmentations. All of the group members benefit from our continuing interactions with Dr. Paul Merkel. We are also delighted to work with Dr. Samir Farid–a long standing collaborator–on a range of research projects.

Richard Eisenberg Tracy H. Harris Professor of Chemistry



RESEARCH INTERESTS

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

CONTACT

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It has been an eventful year for RICH EISENBERG, both professionally and personally. Research on the light-driven generation of hydrogen from aqueous protons - the reductive side of the water splitting reaction - has progressed well with several important accomplishments during the year. Rich feels a touch of irony that after 40 years of working with platinum metal compounds, he is moving to develop hydrogen generating systems that have no noble metals in them. This began with efforts by graduate student PINGWU DU (PH.D. '09) and undergraduate KATHRYN KNOWLES (B.S. '08), which found that certain cobalt complexes can function as catalysts for hydrogen generation from water in photochemically-driven systems. However, in those systems the photoactive element was a platinum complex of the type studied by the Eisenberg group previously. The observation of catalysis by Co complexes was followed up by work of postdoctorals **TED** LAZARIDES (POSTDOCTORAL FELLOW '09) and Theresa McCormick who found that organic dyes can also drive the reaction if they have heavy atom substituents to promote intersystem crossing in the dye excited states, which would then allow for electron transfer chemistry rather than simple fluorescence and non-radiative decay. In these efforts, they were aided by visiting graduate student Genggeng Luo from Xiamen, China.

Rich and Marcia Eisenberg at the Great Wall of China



A second research project involves the use of cationic iridium(III) complexes with labile binding sites as electrophilic catalysts for the Nazarov cyclization and other cationicly driven reactions. This work is being done in collaboration with colleague Alison Frontier and was recently given a vote of support with a research grant from NSF. The parent Ir(III) cationic complex proved invaluable as a catalyst for the Nazarov cyclization in the Merrilactone synthesis published by Alison Frontier in 2008. Second year student Tulaza Vaidya and postdoc Jing Zhang are moving the project forward with efforts to develop and use chiral catalysts and even more reactive cationic systems.

The final project under study in the Eisenberg laboratory relates to the synthesis of new luminescent copper(I) complexes as possible dopant emitters in OLED devices. This work, which is supported by NSF, is based on a collaboration with Kodak Research Laboratories which is actively pursuing this area. Graduate student Jerry Manbeck and postdoctoral researcher Marco Crestani are making new Cu(I) complexes that are neutral in charge, thermally stable for vapor deposition, photoluminescent and reversibly redox active as likely candidates for further study. They have also been aided in this work by undergraduate researcher David Farkas who has been successful in preparing new compounds that satisfy the criteria mentioned above.

Travel is always a big part of the year for Rich and this year was no different. In addition to the annual ACS Meetings (Philadelphia, Salt Lake City) and the ACS Editors Conference which Rich chaired this year (San Diego), there were a number of other meetings and seminar trips of note including invited lectures at the Osaka Forum 2008 on Bio-Environmental Chemistry in San Francisco, the Inorganic Reaction Mechanisms Gordon Research Conference in Galveston, the Inorganic Gordon Research Conference in Biddeford, Maine, and the COST-35 Workshop on "Dithiolenes and Non-innocent Redox-active Ligands" in Vravronas, Greece. However, the highlight of the year was a nearly four-week trip in April to China with his wife Marcia that began with personal touring for ten days and ended with visits to nine universities and institutes in Xiamen, Shanghai, Nanjing, Wuhan, and Beijing. In addition to lectures presented on making solar hydrogen, Rich talked with faculty and students about publishing in *Inorganic Chemistry* and other ACS journals. China is now the largest foreign contributor to ACS journals and to *Inorganic Chemistry* in terms of papers published. Rich was joined in this part of the trip by two of his Associate Editors, and the discussions were stimulating. In addition, he held a regional Editorial Advisory Board Meeting at Peking University for Asian members of the *Inorganic Chemistry* EAB, followed by a great Peking duck banquet (one of several he enjoyed).

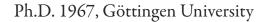
Inorganic Chemistry continues to do extraordinarily well. The most recent Thomson Scientific report of journal impact factors and citations shows *IC* to be at the top of its class with more than 68,356 citations and a record high impact factor of 4.147. This success is a testament to the hard work by the journal's Associate Editors and the journal assistants around the country. Rich is grateful for the tireless efforts put in by Arlene Bristol and Kirstin Key-Campbell in the Editor-in-Chief's office, and is happy to note that Marcia is also filling in on journal business as the work dictates.

Group comings and goings were particularly notable this year as graduate students **PAUL JAROSZ (PH.D. '09)** and **PINGWU DU (PH.D. '09)** successfully finished their Ph.D. studies to move on to the next phase of their careers as independent scientists. They, along with graduate student **JAKE SCHNEIDER (PH.D. '08)**, who finished last May, have moved onto postdoctoral studies: Jake at York University in England working with Robin Perutz, Paul at RIT working on a materials science project that he thoroughly enjoys, and Pingwu at MIT doing research with Steve Lippard. Ted Lazarides has also finished his postdoctoral work and returned to his native Greece to fulfill his national military obligations and undertake new research on solar energy conversion. During the year, three new postdoctorals commenced research in the Eisenberg laboratory: Jing Zhang from Nanjing University via the Weizmann Institute of Science, Marco Crestani from Mexico City and Universidad Nacional Autonóma de México and Theresa McCormick from Queen's University in Canada, who has come to Rochester with a prestigious NSERC Fellowship. Jing is working on the research project involving electrophilic catalysts done in collaboration with the Frontier group, Marco is synthesizing and studying new luminescent Cu complexes and Theresa is picking up the project on the photogeneration of hydrogen. They join continuing graduate students Jerry Manbeck and Tulaza Vaidya in their efforts.

Finally, Rich is grateful and elated by his recent election to the American Academy of Arts and Sciences. He feels that in addition to being a genuine honor, it will also be a privilege to participate in Academy activities that address important societal questions.

Samir Farid

Research Professor





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. Of particular interest in this year's work is a reevaluation of long-standing interpretations of photoinduced electron transfer rates. This work has provided a different view that will change currently accepted convictions. He finds the collaboration with several friends and colleagues to be stimulating and importantly, most enjoyable.



The George Eastman House

James M. Farrar Professor of Chemistry



RESEARCH INTERESTS

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

CONTACT farrar@chem.rochester.edu

JIM FARRAR's interest in crossed beam studies of low energy ion-molecule reactions continues, and he looks forward to beginning a new series of studies on ion-radical reactions using imaging techniques in the near future.

Jim continues to work with the McNair program and Kearns leadership center, along with the Office of Minority Student Affairs, to provide academic assistance to minority students interested in pursuing careers in science. For the fourth year, Jim taught a special summer course, this time on "Problem-Solving Methods in Chemistry," through the College's Early Connection Opportunity (ECO) program. This activity has established a strong connection between Chemistry and University efforts to support minority student success in the sciences. Also for the third year, Jim continued to serve as the director of the Graduate Assistance in Areas of National Need (GAANN) Program in Chemistry.

Two 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.

This past year has been a significant one for both Jim and his wife Kathy, with the birth of their first grandson, Callum James Hermes, on August 30, 2008. Callum and his parents live in New York City, and the grandparents have kept the Thruway busy with trips to check up on his progress.

Martin Brewer Anderson, First President of the University of Rochester, 1853-1888



Rudi Fasan Assistant Professor of Chemistry



RESEARCH INTERESTS

Bioorganic chemistry; chemo-enzymatic synthesis and designed biosynthesis; enzyme engineering and protein directed evolution; study of natural product biosynthetic pathways; chemical biology.

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It has been an exciting first year for **RUDI FASAN** and his new research group on the fourth floor of Hutchison Hall. After turning the shiny and empty space of HH409 and HH411 into a fully functional (and less shiny) research lab by the end of 2008, the Fasan group has steadily grown in subsequent months to include two postdoctoral fellows, four graduate students, and four undergraduate students by Summer 2009.

Our efforts during this year have focused on getting our major research projects off the ground. Our research interests 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 is 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 developing new synthetic approaches to access non-activated C-H bonds in a variety of organic scaffolds such as synthetic building blocks, drugs and natural products. A first demonstration of the synthetic utility of this approach was published in Nature Chem. Biol. early this year, where we applied this strategy to carry out selective fluorination of unactivated sites in small molecules at a preparative scale. Postdoc Kaidong Zhang and UR undergraduate Shady El Damaty are now working on expanding the scope of this approach to complex natural products as well as other types of chemical transformations. The recent acquisition of an Ultra Fast HPLC and a robotic system for automated liquid handling are expected to ease their efforts towards these goals. Shady's work, initiated in early spring of 2009 and continued over the summer thanks to a McNair scholarship, have recently enabled the development of a very convenient and inexpensive cofactor regeneration system to drive our small- and large-scale P450 reactions. To our delight, this research experience has motivated him to pursue a double major in Chemistry and Neuroscience.

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The Fasan Group, Summer 2009

Front row, from left: Shady El Damaty, Helen Kraye, David Condon, Jessica Smith, and Francesca Vitali Back row, from left: Kaidong Zhang, John Frost, Steve Archer, Jacqueline Zaengle, Satyanarayana Maraganis, and Rudi Fasan



A second major project ongoing in our lab is the development of chemo-biosynthetic routes for the production of large and diverse libraries of small molecules in bacteria. The pursuit of this challenging and multifaceted project requires joint synthetic, protein engineering, and protein chemistry efforts. First-year graduate student Jessica Smith (RIT) and postdoc Satyanarayana Maragani have begun tackling some of the synthetic challenges of this project. In June, Jessica was awarded an NSF Graduate Student Fellowship which will support her research for the next three years. Our heartiest congratulations go to her for this prestigious award. Parallel synthetic efforts were undertaken by UR undergraduates Steven Archer (a BME junior) and RUTH SCOLES (B.A. '09) who spent the spring semester in the lab as part of an independent research course (CHM 395). After graduation, Ruth joined the DC Teaching Fellows to teach high school chemistry. Supported by a Mc-Nair scholarship, Steve has continued working in the lab over the summer and was successful in completing the synthesis of his target molecule with excellent yields and at multi-gram scale. The synthetic crew has been recently joined by two incoming graduate students, John Frost (Canisius College) and David Condon (Penn State). John is exploring the possibility of modulating the catalytic properties of P450 enzymes using non-natural amino acids, while Dave is developing a method to

produce cyclic conformationally constrained peptides in living bacteria.

The protein chemistry/protein engineering wing of the group is also expanding. UR undergraduate Rajesh Ravikumar and Jacqueline Zaengle (REU student) worked hard over the summer and made important progress in P450 engineering projects. Senior researcher Francesca Vitali is laying the foundation for the study of the biosynthetic pathway of a plant natural product, and incoming graduate student Helen Kraye (Doane College) is engineering novel enzymes for incorporating fluorine into organic molecules.

In Fall 2008, Rudi taught the graduate course Bioorganic Chemistry and Chemical Biology (CHM 437) for the first time and enjoyed interacting with the little crowd of graduate and upper-level undergraduate students of diverse backgrounds that populate this course. During the summer of 2009 Rudi gave presentations at the Bioorganic Chemistry Gordon Conference and the 238th American Chemical Society National Meeting, where he chaired a session of the Organic Chemistry Division. Other professional commitments during the past year included serving as Phase I reviewer for the NIH 2009 Challenge Grant initiative.

Alison J. Frontier

Associate Professor of Chemistry

Ph.D. 1999, Columbia University



RESEARCH INTERESTS

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

CONTACT

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Professor **ALISON FRONTIER**'s research program is devoted to the planning and execution of syntheses of biologically and structurally interesting natural products. The study of Nazarov cyclization continues, focusing on applications in total synthesis, asymmetric cyclizations, and unusual rearrangement chemistry. The development of an efficient method for the diastereoselective hydrogenation of pyrroles is ongoing, a project that has been carried out by Chao Jiang, who defended his Ph.D. thesis in August. Finally, progress toward the synthesis of two interesting terpenoid natural products, phomactin A and norcembrenolide and related natural products, are also underway. The group has made interesting inroads toward the syntheses of natural product targets this year. The rocaglamide saga was successfully concluded this year, due to the heroic efforts of **JOHN MALONA (PH.D. '08)** and **KEVIN CARIOU (POSTDOC-TORAL FELLOW '09)**. Kevin was also involved in the total synthesis of phomactin A, a PAF antagonist with an unusual macrocyclic structure. Since Kevin's departure in early May, Jen Ciesielski (a second-year student) has capably taken the reins of the project. Chao Jiang has continued his efforts toward the synthesis of tetrapetalone A, using a strategy that begins with Nazarov cyclization and then slithers into mysterious territorymore on that next year, we hope! We continue to study rearrangement chemistry that occurs during Nazarov cyclization (Eric Theiste, second-year student), the behavior of Lewis acidic Ir(III) complexes (in collaboration with the Eisenberg group; Tulaza Vaidya, second-year student), and have completed a study of iodide-initiated aldol cyclization chemistry begun by **DAN CANTERBURY (PH.D. '07)** and completed by Jen Cieselski.

In the fall, two first-year graduate students joined the group. Josh Brooks is beginning a new project focused on the design and execution of a biomimetic strategy for the synthesis of an interesting family of bioactive cembrenolide natural products. William Spencer is studying an interesting variant of the Nazarov cyclization, initiated by oxidation of an allenol ether. Inspired by the key step of the rocaglamide synthesis, this project will give us the opportunity to examine chiral memory effects in electrocyclization. **RYAN DALY (M.S. '09)** earned a Master's degree last May through the 5th year Master's program, doing research with Chao Jiang on hydrogenation of pyrrolic alpha-ketoesters. In mid-June, Abdallah Bitar successfully defended his Ph.D. thesis, and has returned to his studies toward the M.D.

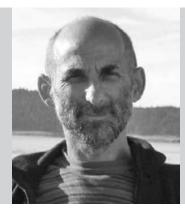


Alison Frontier at the 2009 Chemistry Diploma Ceremony

Joshua L. Goodman

Professor of Chemistry

Ph.D. 1984, Yale University



RESEARCH INTERESTS

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

CONTACT

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



Patrick L. Holland Associate Professor of Chemistry



RESEARCH INTERESTS

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

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The last year has been another great one for **PATRICK HOLLAND** and his coworkers, who continue their exciting organometallic and bioinorganic chemistry research using iron and cobalt complexes. We were happy to celebrate the first publications from third-year students Tom Dugan and Karen Chiang, who have also received awards. Karen was the recipient of travel awards from the ACS Women Chemists Committee and from the UR GWIS (Graduate Women in Science) to present her results at the National Meeting of the American Chemical Society. Tom was the recipient of an Elon H. Hooker Fellowship which began in September 2009, an honor that recognizes his research productivity and academic excellence.

Graduate students Meghan Clark and Ryan Cowley also joined the publication parade. Ryan wrote two papers, one on a new catalytic reaction that transforms azides into carbodiimides or isocyanates, and another on an unusual complex with a radical attached to a metal. Meghan fortuitously crystallized the useful reducing agent Cp*₂Co, and she together with crystallographer Bill Brennessel wrote it up for a crystallography journal. Not only was it accepted in record time (6 hours from submission to acceptance), it was featured as a cover article! Senior students were in on the publication action as well. Sally Rocks wrote a paper describing a new class of ligands that she has pioneered in the group, and presented her work at a National ACS Meeting. Keying Ding submitted two communications on new cobalt-nitrogen chemistry which will appear in J. Am. Chem. Soc. in July and August 2009. Keying successfully defended her doctoral thesis in May 2009, and will be moving to a postdoctoral position with Prof. Connie Lu at the University of Minnesota. Keying has been a big success at isolating interesting complexes incorporating H₂ and N₂, and we applaud her accomplishments that led to a Ph.D.

Holland Group snowtubing in Winter 2009



Another departure was **BEN DIBLE (POSTDOCTORAL FEL-LOW '09)** who has been in the group since 2006. Ben has been a fixture in the lab due to his exemplary work ethic, expertise on organic methodology, and excellent taste in martial-arts movies. He has moved to a postdoctoral position at the University of Pennsylvania with Prof. Amos Smith. We also have a new face in the group: first-year student Sarina Clancy joined us, and we enjoy her infectious verve for chemistry.

Although he is not formally a group member, we owe a huge debt of gratitude to Bill Brennessel, our friend and departmental crystallographer, for his many contributions to our research success. His enthusiasm and expertise have led to his inclusion as a coauthor on numerous manuscripts from our research, and everyone enjoys working with him. We especially recognize Bill's being awarded a Sandra Beach Award by the Department for his efforts including the institution of a departmental "grill-out" next to our lab every Tuesday.

Pat continued to spread the word about group results. He published an invited review in *Accounts of Chemical Research* that describes the group's work on three-coordinate iron complexes. He gave ten invited lectures at other universities including Johns Hopkins, Penn, Texas, and Toronto, and also presented talks at the two biggest bioinorganic chemistry conferences, the Metals in Biology Gordon Conference and the International Conference on Biological Inorganic Chemistry. Pat was also named to the Editorial Board of the *Journal of Biological Inorganic Chemistry*.

Group alumni continue to thrive as well. JEREMY SMITH (POSTDOCTORAL FELLOW '03) was promoted to an associate professor with tenure at New Mexico State University, and was awarded a 2009 Camille Dreyfus Teacher-Scholar Award that recognizes his outstanding research accomplishments as an independent faculty member. Jeremy visited Rochester in the fall of 2008 for an invited seminar, and the new generation of students was able to meet the author of our first ground-breaking research. JAVIER VELA (PH.D. '05) started his independent academic career in July 2009 as an assistant professor at Iowa State University, where he undoubtedly will be a huge success. PAM BARRETT (B.S. **'06)** is beginning Ph.D. work in Oceanography at the University of Washington in the fall of 2009. We congratulate SAVARIRAJ KINGSLEY (POSTDOCTORAL FELLOW '03) and YING YU (PH.D. '07) on their new offspring...they are out in the world demonstrating the productivity of UR researchers!

William D. Jones Charles F. Houghton Professor of Chemistry



RESEARCH INTERESTS

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

CONTACT jones@chem.rochester.edu

The **JONES** group has been actively pursuing organometallic chemistry and catalysis. We had no new graduate students this year, and one student graduated this spring. We have a new postdoc in the group, Dr. Taro Tanabe from Kyoto University. We also have one new M.S. student and two undergraduates involved in their senior thesis research, so the lab is near full capacity with 11 people. Our research is now 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. The group continues in a leadership role in the Center for Enabling New Technologies through Catalysis (CENTC), in which the group has collaborative research projects that are exploring new electrophilic C-H activation catalysts and new direct routes to aromatic amines from benzene. Bill continues as Associate Editor for the Journal of the American Chemical Society for a seventh year, where he handled close to 500 manuscripts a year. Last year he lectured in Florence (ISHC), Rennes (ICOMC), Hamilton, Ontario, UCLA, UCI, UCSD, and the Technion and Weizmann Institute in Israel. During the fall of 2008, Bill was a JSPS Fellow and spent three weeks lecturing at ten Universities in Japan. One graduate student completed his degree, LING LI (PH.D. '09), and is now a postdoc with Jack Norton at Columbia.

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.

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 Naciónal Autonomas de México.

Bill has also been invited back to Japan this fall to speak at the 2nd International Symposium on Synergy of Elements in Sapporo, and will also be a keynote lecturer at the 2nd Asian Conference on Coordination Chemistry in Nanjing, China. He is also a member of the International Scientific Committee for the International Conference on Organometallic Chemistry, 2010. 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.

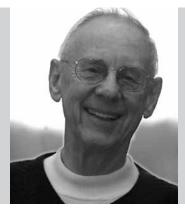
One final newsworthy item, Bill was selected to receive a 2009 Edward Peck Curtis Award for Excellence in Teaching. This award was presented at the University's undergraduate commencement ceremony on May 17th. Thanks to all of you who made this possible.

The Department and Jones Group celebrate the Cope Award



Jack A. Kampmeier

Professor Emeritus of Chemistry



RESEARCH INTERESTS

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

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In previous Newsletters, I have commented on my collaborative work with Frank Saeva (Kodak) and Torben Lund (Roskilde University, Denmark). In 2008, we brought that project to completion by submitting "Regioselectivity in the Reductive Bond Cleavage of Diarylalkylsulfonium Salts: Variation with Driving Force and Structure of Sulfuraryl Radical Intermediates" to *JACS*. This work had its origins in key observations by another long-time colleague, Don Wedegaertner, during his sabbatical at Rochester in 1995. I am reading page proofs for *JACS* as I write these notes.

The Workshop year got off to a good start with the James Flack Norris award ceremony in Boston last November (see last year's Newsletter article or http://www.chem.rochester.edu/news/ news.php?id=11). The local program took a big step forward with the introduction of Workshops in two core courses in the MBA program in the Simon School of Business. The first reports from faculty and peer leaders are enthusiastic and preparations are underway for a second year in 2009-10. This experiment is the first intramural transfer of the workshop program to another college and a significant implementation in the social sciences. (Coincidentally, Mark Zupan, the Dean of the Simon School is the son of **MARIA ZUPAN (PH.D. '64)** with W. D. Walters in Chemistry).

In 1995, I got tapped to lead the search committee to find a new Dean of the River Campus libraries. One thing leads to another and in this case, to a continuing involvement with the Friends of the University of Rochester Libraries and a two-year term as President of that organization (2007-2009). A colleague noted that volunteer activities bring rewarding opportunities to make new friends; that was certainly true in my case as I became involved with new colleagues and programs in our superb research libraries. I was predisposed to these activities by a long-term tutorial from Arleen Somerville and Andy Kende about the power of librarians and libraries.



Owl Sculpture atop the Cupola of Rush Rhees Library

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 kende@chem.rochester.edu

Now living full time in Scottsdale, AZ with his wife Frances, Professor **ANDREW KENDE** and Mrs. Kende returned to Rochester for a week in mid-August, then continued on to the 238th American Chemical Society National Meeting in Washington, DC. As a Director of Organic Reactions, Inc., Prof. Kende participated in the August 17th annual meeting of the O.R. Board of Directors as that book series expands into a full electronic version readily accessible to organic chemists worldwide.

Prof. Kende is now a proud member of the Central Arizona Section of the American Chemical Society. In January 2009 he

hosted NORITADA MATSUO (POSTDOCTORAL FELLOW

'88) a Research Fellow at Sumitomo Co., on Dr. Matsuo's most recent trip to Phoenix. Prof. Kende looks forward to visiting the UR Chemistry Department in March 2010 to enjoy the fifth "Andrew S. Kende Distinguished Lecture Series", to be delivered by Prof. Dean Toste of the University of California at Berkeley during the week of March 29, 2010. Prof. Kende invites former UR graduate students, postdoctoral fellows and colleagues to contact him via his UR email address (kende@chem.rochester. edu) if they plan to be in the Phoenix area in the coming year.

Todd D. Krauss

Associate Professor of Chemistry

Ph.D. 1998, Cornell University



RESEARCH INTERESTS

Physical chemistry; synthesis and characterization of nanometer scale materials and devices, 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 this past year produced more productive members of society. Congratulations to **KATIE LEACH (PH.D. '09)**, who successfully defended her thesis in April. Katie was highly sought after even in this tough job market, and she is now working for Advanced Concepts and Technologies International directing their carbon nanotube and graphene research program. **ZHIHUI BAN (POSTDOCTORAL FELLOW '09)** departed the group in February after completing toxicology studies on whether nanoparticles can cross the blood-brain barrier. Zhihui is currently in Boston with his two new children and we expect has his hands full! Congratulations are also in order for Chris Evans, who won selection to participate in the 59th meeting of Nobel Laureates in Lindau, Germany this summer, as well as a 2009 SPIE Scholarship in Optical Science and Engineering. Chris also discovered the first general mechanism for synthesis of semiconductor nanoparticles, which allowed him to produce the same amount of product with 1000 times less starting material! This is an important discovery and actually has caught the interest of several large companies that make nanoparticles.

Postdoctoral fellows Xiaoyong Wang, Andrea Lee and graduate student Lisa Carlson also had a break-through discovery: they were able to increase the emission efficiency of carbon nanotubes in solution by 10 times! Their discovery will likely lead to many uses of nanotubes for applications requiring a very stable source of infrared light. Shujing Wang and postdoctoral fellow Marat Khafizov finally succeed in generating multiple electrons from a single photon of light in carbon nanotubes! Someday this "buy one get one free" type process may allow for more efficient solar cells. Also, Amy Ensign, Dr. Andrea Lee and Wesley Asher, all co-advised by Prof. Kara Bren, together had great fun exploring various aspects of protein folding on the single particle level.

Todd Krauss and Daniel Weix



Helen Wei spent last year trying to make large batches of the "special" nonblinking quantum dots with potential for vastly improved lasers and optical amplifiers, while Jenneke Jalink was working hard to make vertically aligned carbon nanotube arrays with potential relevance for the production of hydrogen from solar energy. Julie Smyder dove deep into the fluorescence of single clusters of semiconductor nanoparticles that are less than 100 atoms total, while Jack Calcines spent the better part of last year discovering a new way to grow elongated semiconductor nanoparticles called quantum rods with the highest aspect ratio reported to date for this chemical system. Jack and Julie should have their contributions in print very soon – congratulations! The group is delighted to have added a couple of new students to the mix: Fen Qiu and Brad Loesch who are working in the nano-crystal and nanotube areas, respectively, as they get going.

During the summer the group hosted two undergraduates from the University of Rochester: Matt McKay and Don Polaski. They have been with the group through the entire year and are enjoying not taking any hard UR classes so they can focus fully on research.

Finally, Todd was pleasantly very busy this year between a new graduate course on the electronic properties of molecules to materials and writing up several "important" results coming from the hard work of the group. However, he still found time to organize the first University conference on nanomaterials, "Nano-Symposium 2009", which was great fun for those who attended.

Robert W. Kreilick Professor Emeritus of Chemistry

Ph.D. 1964, Washington University



RESEARCH INTERESTS

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

CONTACT

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ROBERT KREILICK is enjoying his second 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. Last year, 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.

Spring in Highland Park, adjacent to the River Campus



Thomas R. Krugh

Professor of Chemistry



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.

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Our summer National Science Foundation Research Experience for Undergraduates (NSF REU) program continues as one focus of **TOM KRUGH**'s activities. The 2009 summer program includes 17 UR students along with seven students from other schools. NSF renewed funding for our REU program and this is the first year in a new three-year cycle. You may recall from past years that we also had six high school teachers each summer, funded also by the NSF grant. NSF, unfortunately, decided to cancel the program that funded high school teachers. The heart of our program remains focused on our summer undergraduate research participants and, in that respect, we are delighted funding is continuing for another three years. Tom traveled to Dublin, Ireland last December to participate in a National Science Foundation of Ireland panel to review proposals for summer research programs. The weekend after returning from Dublin, Tom and Rody journeyed to Palo Alto for a 75th birthday celebration of John Baldeschwieler, who was Tom's postdoctoral adviser (July 1969 to July 1970). It was enjoyable to catch up with 'old' friends from Tom's postdoctoral year at Stanford.

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.

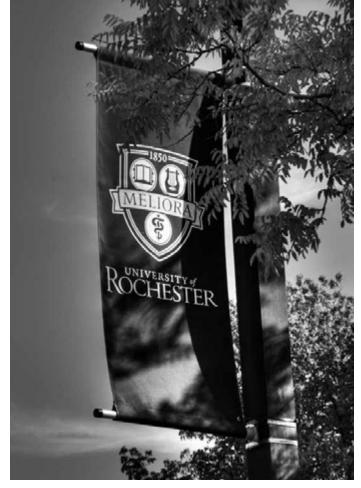
CONTACT

mccamant@chem.rochester.edu

The **MCCAMANT** group has been continuing to grow and get better data. In May 2008, undergraduate **BRENDON LYONS (B.S. '08)** graduated but decided to continue with us for another year while pursuing a Master's degree. We were also lucky enough to have junior Randy Mehlenbacher continue to work with us this year. We've had exciting collaborations studying the ultrafast dynamics of a number of platinum compounds that the Eisenberg group has assembled, as well as a fun collection of charge-transfer and excimer dimers from the Rothberg group. Third-year graduate student Kristina Wilson and Brendon received the physical chemistry graduate student poster award at the fall 2009 ACS meeting. First-year graduate student Einstein Ofotsu Djabeng joined the group this year and will be pursuing studies of DNA photophysics, working with our new post-doc Yong Du. Yong came here after his Ph.D. at the University of Hong Kong, where he worked with another Rochester alum, Prof. **DAVID PHILLIPS (POSTDOCTORAL FELLOW '92)**, who did work with Anne Myers here in Rochester. Dave had a busy spring semester teaching CHM 458, Molecular Spectroscopy and Structure and CHM 460, Chemical Kinetics, in addition to CHM 231, Chemical Instrumentation, in the fall. Last summer, Dave and his group were excited to learn that two research proposals submitted last year were granted. The American Chemical Society's Petroleum Research Fund will support a study to probe vibrational coupling in aromatic hydrocarbons and metallocenes using femtosecond stimulated Raman spectroscopy (FSRS). Dave was also thrilled to receive an NSF CAREER award. With this award the McCamant group will receive significant funding over the next five years from the NSF Experimental Physical Chemistry program in support of their research to develop femtosecond stimulated Raman spectroscopy (FSRS) to study ultrafast processes in photochemistry and photobiology. Research is progressing well on all fronts and we're enjoying life, science and the camaraderie of the basement in Hutchison Hall.

Colleen Kellenberger (B.S. '09) and Dave McCamant





Banner with University Shield

John S. Muenter Professor Emeritus of Chemistry

Ph.D. 1965, Stanford University



RESEARCH INTERESTS

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

CONTACT

muenter@chem.rochester.edu

JOHN MUENTER is enjoying retirement but he is still active in the Department, coming to seminars and attending Dave McCamant's research group meetings. Spectroscopy collaborations are continuing with Carlo Callegari and with MARK MARSHALL (B.S. '75) and Helen Leung. There are no new papers this year, but two should appear in the coming year. One will describe the last work from the long collaboration with Tom Rizzo in Switzerland. The main author on this paper is Andrea Callegari, Carlo's identical twin brother, and the paper describes quantum beat measurements used to observe electric dipole moments of very high energy vibrational states of water. The second paper is from the Technical University in Graz, Austria, with Carlo, and describes ESR measurements on single alkali metal atoms adsorbed on the surface of liquid helium nanodroplets. This work was done in the old Rochester molecular beam apparatus since it moved to Graz.

The Erie Canal



Bradley L. Nilsson

Assistant Professor of Chemistry



RESEARCH INTERESTS

Bioorganic chemistry and chemical biology, protein engineering and quaternary structure, amyloid peptides and proteins, chemical synthesis of proteins.

CONTACT

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During the last year the NILSSON group has continued efforts to understand the interactions that lead to amyloid formation in self-assembly peptides. Our work has focused on: 1) the characterization of noncovalent side-chain interactions that give rise to protein aggregation and fibril formation, with an emphasis on the Alzheimer's disease amyloid- β peptide and on designed β -sheet forming peptides; 2) the design of proteins that self-assemble under reductive control; 3) the development of new methods for the chemical synthesis of proteins using oligonucleotide-templated strategies. This research has spawned new research projects, including the exploration of small molecule self-assembly for hydrogel formation. An amino acid-derived moiety was discovered that undergoes rapid self-assembly in water to promote gelation and we are exploring biomedical applications of these materials for wound healing and cell growth. In addition to the DuPont Young Professor Award and an Alzheimer's Association New Investigator Grant, the Nilsson group was successful in applying for a Doctoral New Investigator Grant from the ACS Petroleum Research Fund.

Membership in the Nilsson group has continued to grow and the existing members have been very productive in the last year. Timur Senguen has focused on probing the self-assembly of an amyloid- β derived peptide by incorporating hexafluoroleucine and has also made significant progress in understanding the thermodynamics of hydrophobic vs. aromatic interactions in this peptide. Charlie Bowerman is studying the self-assembly of designed peptides that contain nonnatural amino acids and how to control the self-assembly of these peptides using a reductive trigger. Todd Doran continues to work on templated peptide ligation and photocontrol of amyloid- β aggregation, and has also expanded his research effort to include a study of the diabetes type II peptide, the islet amyloid polypeptide. Derek Ryan is probing the effect that highly fluorinated aromatic amino acids have on amyloid-β aggregation and has discovered that small, fluorinated molecules under highly efficient self-assembly give hydrogel materials. A new postdoc, Beth Anderson, has joined the Nilsson group and has initiated several research projects, including an effort to design MRI contrast agents to be used in the diagnosis of Alzheimer's disease. Beth recently welcomed the addition of new daughter, Evelyn, to her family has well! John DiMaio (Alfred University) and Ria Swanekamp (SUNY Brockport) joined the Nilsson group in the last year as well. John is studying peptide self-assembly and preparing novel nonnatural amino acids to incorporate into self-assembling peptides and Ria is working on new synthetic methodology for the catalytic asymmetric synthesis of amino acids. Naomi Lee took a brief leave of absence last year during which she joined the Army National Guard, requiring her to undergo basic training and officer's training. She's expected to recommence her Ph.D. studies in the fall.

NADIA BYRNES (B.S. '09), JOHN OAKFORD (B.A. '09), and CELINE LEUNG (B.S. '09) are three undergraduates who have worked in the lab over the last year and all have recently graduated. Nadia will be attending Ohio State in the fall to study food chemistry, John will be in Rochester for one more year as part of the Take 5 program, and Celine will be applying to medical school. They are all very talented and have contributed productively to a variety of projects in the group. We're confident in their future success! Sam Anderson, a sophomore who took Chemistry 172Q from Brad (and excelled) last year has joined the lab and is completing REU research during the summer studying small molecule self-assembly.

Brad once again taught the second semester of Quest Organic Chemistry (CHM 172Q). The students have continued to be engaging and exciting to work with. This year, Brad left Bioorganic Chemistry behind and added another Quest class to his teaching responsibilities, Chemistry 173Q, the first semester Quest organic chemistry lab. The lab course represented a new challenge and provided a great opportunity to meet the Quest students prior to 172Q in the Spring semester.

As research in the Nilsson group has matured, life has become very busy. A summer of meetings (four and counting), grant-writing (three and counting), and paper-writing has kept us all working hard. We look forward to another year of progress.

Brad Nilsson and sophomore Sam Anderson

Misha Ovchinnikov

Assistant Professor of Chemistry



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.

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MISHA OVCHINNIKOV completed his sixth year of teaching and research in theoretical physical chemistry in the Department of Chemistry at UR. Misha's research primarily focuses on the development of new methods for solving many-body quantum dynamics problems. The Ovchinnikov group is developing effective numerical methods that can calculate quantum mechanical time evolution based on its semiclassical representation by classical trajectories. During the past year, research has been focused on the development of a new method, the so-called Coherent State Path Integral (CSPI) semi-classical dynamics or "complex trajectory" method. The Ovchinnikov group successfully applied this method to a number of test problems and is now using it to solve exciting problems in quantum mechanics.

Lewis J. Rothberg

Professor of Chemistry

Ph.D. 1983, Harvard University



RESEARCH INTERESTS

Physical chemistry: metal nanoparticle-enhanced molecular spectroscopy, biomolecular sensing, photophysics of conjugated organic materials.

CONTACT

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LEWIS ROTHBERG's group is growing once again and sometimes Lewis has a hard time keeping up with the rapid pace of progress. Senior graduate students Steve Paquette and Millard Wyman are both generating exciting new data. Steve is both deepening our understanding of how metal-nanoparticle interactions with molecules change their spectroscopy and demonstrating practical consequences such as enhanced energy transfer between chromophores and suppression of photobleaching in dyes. Steve's energy has allowed him to carry off another project in addition to his thesis work, doing what we think will be landmark studies in how packing of conjugated chromophores affects their photophysics. That work has been made possible by terrific collaborators in the Department (Justin Rhinehart and Prof. Dave McCamant) and at University of Delaware (Onur Kas and Prof. Kristi Kiick). Millard has initiated collaborative work with Prof. Ulli Scherf at Universität Wuppertal to quantify charge generation and recombination processes in conjugated polymeric systems of interest for organic electronics. Both continue to impress with their independence and fearlessness in the lab and are beginning to present the fruits of their labor at professional meetings and in publications. Meanwhile, **ED NELSON (PH.D. '09, PHYSICS)** successfully defended his thesis concerning the kinetics and thermodynamics of DNA adsorption. It was both experimentally and theoretically challenging work and has compelled us to completely reassess our thinking on the reasons single-stranded and double-stranded DNA behave so differently. Several more graduate students have joined the group and are bringing new energy and talent. Xiao Wang from Biophysics and Structural Biology, a program to which Lewis was recently appointed, is continuing TINGJUAN GAO's (PH.D. '04) work on reflective interferometry and applying it to interesting biomolecular science problems. We received a grant to build a prototype instrument and we are publicizing the advantages of the method to facilitate it becoming widely used for label-free sensing. Chi-Sheng Chang, a materials science student with synthetic interests and experience has begun a project to further the group's work on investigating how plasmon enhancement by metal nanoparticles can be used to address problems in solar photovoltaic technology. Kelly Sassin from Physics is studying mechanistic issues in organic light-emitting diodes and photovoltaics in collaboration with Dr. Ralph Young and Dr. Al Marchetti whom we are blessed to have as resident scientists who contribute heavily to both our research and educational missions.

Ben Martin is writing up his fifth-year M.S. project and we are happy he has decided to continue in our Ph.D. program. His research has a lot of momentum now and we are anticipating exciting results in single chain polymer spectroscopy. He is also working on several biological applications of single molecule spectroscopy with Prof. Alan Smrcka from the medical school. A cadre of talented undergraduates have worked with us during the year including **ZANNY STWERTKA (B.A. '09)** (who also decided to enter our Ph.D. program), Kishan Tarpara and **MATT MERRIMAN (B.S. '09)**. Matt and Kishan both did largely synthetic chemistry, a brave undertaking in the Rothberg group, but something Lewis has come to appreciate very much as integral to our progress. Lewis was privileged to be able to present Matt with his degree and pleased to see him on his way to medical school after a year of work.

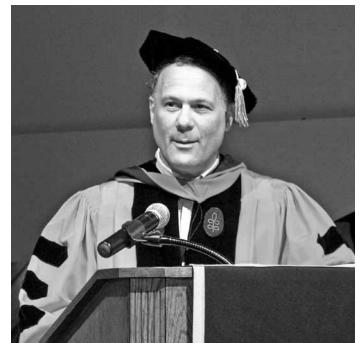
Growing and shaping the energy research and materials program on campus are two of the prominent initiatives on campus now and our group is in the middle of both efforts. Lewis presented some of the group's work on plasmon-enhanced organic solar cells at the Energy Research Initiative meeting in April and helped to co-organize the Nanomaterials Symposium in May. We are working closely with a number of colleagues including Todd Krauss, Ching Tang, Shaw Chen and Philippe Fauchet to bring high profile materials and energy centers to campus. Dean Rob Clark, the new Dean of Engineering, is a strong and aggressive advocate of these programs and there is a universal sense that good things will come of our efforts.

As usual, we hosted several summer students. Janelyn Gonzalez Morales worked on Forster transfer studies with Steve Paquette and Adam Breland with Ben Martin on DNA strand invasion experiments, a collaborative effort with Profs. Doug Turner and **DAVE MATHEWS (PH.D. '02, M.D. '03)**. In addition, David Stelter, a Pittsford high school summer student joined us to study DNA adsorption using Raman spectroscopy. Summer in Rochester is delightful and Lewis hopes to spend much more time in the lab. Lewis taught the graduate quantum mechanics class (CHM 451) for the first time this fall and loved it. He taught the advanced spectroscopy lab (CHM 232) in the Spring under somewhat challenging conditions (on crutches from an Achilles tendon rupture) and was very grateful to James Morris, a super teaching fellow, and Ray Teng who picked up a lot of the attendant slack. Lewis continues to be active both presenting work and organizing professional meetings. This year, he gave seminars at the University of Chicago, University of Connecticut, University of Colorado Boulder and Colgate as well as invited talks at the Society for Information Display meeting and the Optical Probes of Conjugated Polymers meeting. Lewis was also program co-chair for the annual national APS Division of Laser Science/Optical Society meeting and on several other conference program committees.

As mentioned last year, one of the developments from the lab has spawned a commercialization effort and Lewis remains involved in that work. Dr. Barbara Stwertka is doing a sensational job moving that work forward with Rhiannon Gaborski of Diffinity and Lewis is having a blast interacting with them and watching the progress and growth of that effort. Moreover, Barbara has had a huge substantive impact on many projects in the group and her enthusiasm and "can do" attitude have noticeably brightened the environment. The company, Diffinity Genomics, rents space in Hutchison and reached an agreement to license our intellectual property from the University. Diffinity was blessed with a savvy, energetic and charismatic new CEO this past fall, Jeff Helfer, who has enhanced the prospects of success enormously. This should be an exciting and pivotal year for that work.

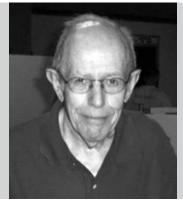
Shelby, Lewis, Charles (6), and Vivian (5) are growing happily. Shelby is doing terrific work at Kodak and thriving in her myriad roles outside of work as well. Charles is enjoying soccer and Star Wars while Vivian is partial to gymnastics and Pet Shop. Lewis' mother, Esther Conwell, was recognized for her contributions to science with an honorary degree from SUNY Geneseo and continues to be active in the department and a source of inspiration to many.

Lewis Rothberg at the 2009 Chemistry Diploma Ceremony



William H. Saunders

Professor Emeritus of Chemistry



RESEARCH INTERESTS

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

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BILL SAUNDERS continues valence bond calculations on elimination reactions. Current computational studies are aimed at providing evidence for the prediction that truly synchronous E2 reactions are rare because they have high energy barriers. I attended the Reaction Mechanisms Conference at the University of North Carolina. Nonscientific activities included visits in June and August to the Stratford Shakespeare Festival in Canada, the latter trip along with daughter Anne and two granddaughters, Zoe and Sara. In July, Dave and Marty Wilson visited Rochester and stayed with me. Dave was a chemistry faculty member during my early years at the University of Rochester. The bicycle trip of the year was to the Andalusia region of Spain in November. We saw many examples of Muslim influence in Seville, Cordoba, and Granada. During the time that they were dominant they were more tolerant of other religions than were the Christians who followed them. Again at Christmas time there were visits from Anne, her two girls, Claude, his wife Gulchin, and stepdaugher Nina. My remaining travel was in early April to North Carolina, where the spring was much more advanced than in upstate New York.

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

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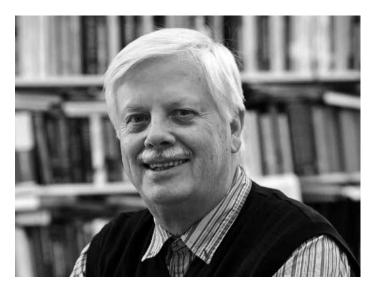
UDO SCHRÖDER's group continued research in radio-chemistry, heavy-ion reaction dynamics, as well as technical R&D. In collaborative experiments with a group from the UR Laboratory for Laser Energetics, interactions of tritriated compounds with metallic surfaces and metal lattices were studied. These processes are of interest to the nuclear power industry. Results obtained from the group's experiments with thermal and RF plasma desorption techniques were presented on several meetings by the involved students and in a peer-reviewed publication.

Technical progress has also been made in the identification of heavy nuclear particles stopping in silicon detectors. A simple

and economical method has been devised to identify such particles based on their time evolved ionization track.

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 theoretical model developed by the group to describe the stability and fission-like disintegration processes of highly unstable, hot nuclei has been extended further. It has been successful in predicting a host of previously puzzling observations in nuclear decay within a cohesive, plausible physical picture. Most recently, the model has been employed to explain the effects of a quantum symmetry leading to certain isotopic regularities ("isoscaling") in the nuclear species produced in statistical disintegration.

Group members presented talks at ACS and APS meetings. Udo gave invited lectures at the New Orleans Seaborg Symposium, the Catania Symposium on Nuclear Symmetry Energy, and the Albuquerque Nuclear and Radiochemistry Workshop, in addition to research seminars in the UR Departments of Chemistry, Physics, and Electrical Engineering. He also presented lectures on energy issues at Rochester and Gettysburg.





Harry A. Stern Assistant Professor of Chemistry

Ph.D. 2001, Columbia University



RESEARCH INTERESTS

Computer simulations in biochemistry and structural biology; signal transduction by Gprotein coupled receptors; computational prediction of protein-ligand binding affinities; algorithms and potential energy functions for large-scale simulation of condensed phase systems; statistical mechanics.

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HARRY STERN's group was sorry to see the departure of postdoc ORR RAVITZ (POSTDOCTORAL FELLOW '08) to Toronto but happy that he has moved on to bigger and better things. He is now an applications scientist at SimBioSys, a company that develops computational chemistry software for drug discovery. In collaboration with Alan Smrcka's lab in pharmacology, graduate student Min-Sun Park (Biochemistry and Biophysics) published a paper a few months ago examining docking methods for the prediction of binding affinities of small-molecule ligands to the beta-gamma heterodimer of the G protein, which has the potential to become a novel therapeutic target. Min-Sun is currently running simulations to examine the mobility of tryptophan residues near the binding surface and to compare with NMR experiments. Grad student Cen Gao has been working on a new method to account for the effects of ligand conformational change when calculating binding affinities. He has a paper submitted to *Biophysical Journal* describing the implementation of the method, tests on simple model systems, and application to examining 233 protein-ligand complexes for which experimental crystal structures and measured affinities are available. The results show that both entropic and enthalpic contributions due to ligand reorganization are important in binding, and accounting for these contributions can provide an improvement in the agreement of calculations with measured affinities. Cen is now working on the most critical part of any methodology for affinity prediction–the force field used to compute intermolecular interactions. He is developing a new model incorporating electrostatic polarizability using the fluctuating charge model, parameterized by fitting to density functional theory calculations of small molecules in both gas and crystalline phases, which represent extremes of the degree of intermolecular interaction. During the spring, Biochemistry and Biophysics graduate student Joshua Horn did a rotation in the group, running molecular dynamics simulations of a small oligonucleotide to examine vibrational relaxation after photoexcitation, which is being studied in Dave McCamant's group. Harry has also enjoyed collaborating with **ILYAS YILDIRIM (PH.D. '09)** in Doug Turner's group on free energy calculations and molecular dynamics simulations of oligonucleotides. Ilyas defended last August and published a paper in the *Journal of Chemical Theory and Computation*.

On the home front Eva and Danny are keeping their parents busy. Eva is on her way to becoming an accomplished visual artist (mixed media) and has a permanent installation on our refrigerator as well as several traveling exhibitions throughout the house. She likes music as well, as long as her dad is not singing it. Much of our parenting time is spent chasing Danny around and trying to take things out of his mouth before he can eat them. The list is extensive and includes not only traditional comfort food such as crayons, chalk, garden soil, woodchips, and sand, but more cosmopolitan tastes including ladybugs (dried), band-aids (used), sticks of butter (straight up), and hand soap. He also enjoys sprinting down our driveway towards Brunswick Street, tearing a hard right, and taking off down the sidewalk towards Park Ave. This is especially rewarding if being chased by a parent and even better, if the parent is yelling.

The Eastman Theatre



Douglas H. Turner

Professor of Chemistry

Ph.D. 1972, Columbia University



RESEARCH INTERESTS

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

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This year's science continued the steady progress in understanding RNA. Jim Hart's paper on NMR Assisted Prediction of Secondary Structure (NAPSS - Doug's favorite hobby) was published. Jim collaborated with Scott Kennedy and **DAVE MATHEWS (PH.D. '02, M.D. '03)** in the Department of Biochemistry and Biophysics and then returned to Medical School. The NAPSS method revealed an unusual 74 nucleotide pseudoknot in a retrotransposon discovered by Tom Eickbush in UR's Biology Department. In collaboration with the Eickbush group, Ela Kierzek and Walter Moss, respectively, provided experimental and bioinformatic support for the pseudoknot and for other conserved secondary structures in a 320 nucleotide segment in five retrotransposons. Walter also noticed an interesting progression in the sequence from a region coding for conserved RNA secondary structure to one conserving both RNA secondary structure and protein sequence to one conserving only protein sequence. Insights into RNA thermodynamics were provided by the Kierzek group's work on locked nucleic acids (LNA) and **GANG CHEN'S (PH.D. '06)** work on CA pairs, which are extra stable in certain contexts. **ILYAS YILDIRIM (PH.D. '09)** collaborated with Harry Stern and the Sponer group in the Czech Republic to test the ability of computational approaches to predict NMR structures previously determined by **JOHN SANTALUCIA (PH.D. '91)**, **MING WU (PH.D. '96)**, Gang Chen, and Scott Kennedy. The bottom line is that computational approaches need to be improved Ilyas graduated with a Ph.D. in Physics and is now a postdoc in the group.

Previous graduates from the group continue to make more than steady progress. MARK BURKARD (PH.D. '01, M.D. '02) started a faculty position in the Cancer Center at the University of Wisconsin, Madison. BLANTON TOLBERT (PH.D. '07) accepted a faculty position at Miami University in Ohio, where he will have access to both an 800 MHz and a 500 MHz NMR. NEEL SHANKAR (PH.D. '08) started a position at the Nixon, Peabody law firm in Rochester, where he is working on patents. SUSAN SCHROEDER (PH.D. '02) at the University of Oklahoma received an NSF Career Award. BRENT ZNOSKO (PH.D. '04) had an NIH grant funded. As a postdoc with Nacho Tinoco at Berkeley, Gang Chen won an award for the best biophysical and structural biology poster at the RNA Society meeting and has accepted a new postdoc position with David Millar at the Scripps Institute in La Jolla. First year students Jonathan Chen and Sal Priore should add to the tradition. Jon was an undergraduate major in Optics at UR and Sal graduated from SUNY Geneseo and is in the MD/PhD program.

Doug presented the group's work at an RNA Ontology Meeting in Berlin, and in talks at Carnegie Mellon, where he was hosted by **BRUCE ARMITAGE (B.S. '88)**, Binghamton University, and the University of Oklahoma, where he was hosted by Susan Schroeder. He also gave a talk at the SUNY Albany Chemistry graduation, where he advised the students to find what they love and then find somebody to pay them to do it. The words made Doug realize how lucky he is. He was also lucky to be called back as a pinch hitter to review training grants for the NIH. One site visit was to Berkeley where he was able to dine with former students Gang Chen and **XIAOYING CHEN (PH.D. '00)** at dinner; **YI LI (PH.D. '97)** and **MING WU (PH.D. '96)** at a late breakfast; and to talk on the phone with **XIAOQI JIAO (PH.D.'95)**, who called the dinner group after getting off a plane at the San Francisco Airport. Doug also spent time with his postdoctoral advisor, Nacho Tinoco. In June, the group welcomed Ela Kierzek to the lab for a summer visit. She will be joined later by Ryszard.

In the Spring, Doug taught part of the Biophysical Chemistry course and all of the Monday, Wednesday, Friday first year Chemistry course. In the latter, he tries to give an assignment that will help students develop their creativity. This year, the assignment was to write a page for an apocryphal book called "The Cold Diet," where the theme is that thermodynamics predicts that eating meals cold provides fewer calories. Unfortunately, many students found relevant web sites, including one with an article called "The Ice Diet." In the future, Doug will have to be more creative to stay a step ahead of Google.

Daniel J. Weix

Assistant Professor of Chemistry

Ph.D. 2005, University of California, Berkeley



RESEARCH INTERESTS

The development of new catalytic methods for organic synthesis with an emphasis on the isolation of potential intermediates and the study of proposed elementary steps. Current interests include transition-metal-catalyzed C-C bond forming reactions; the synthesis of alcohols and amines; enantioselective catalysis; concurrent tandem catalysis and artificial megasynthases.

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Research in **DANIEL WEIX**'s group is in full swing with three students joining the group in 2008: Daniel A. Everson (University of St. Thomas), Michael R. Prinsell (Colgate University), and Ruja Shrestha (Lake Forest College). In addition, we recently welcomed our first graduate student of 2009, Alex Wotal (Hope College). After setting up the labs (located in Hutchison Hall 421 and 422) in record time, we got down to the business of developing new catalytic reactions. In the general area of cross-coupling reactions we now have excellent initial results on several fronts which we hope to communicate this coming year. In addition to the multiple cross-coupling projects, we have several other new reactions that are under development. Every day brings new reactivity it seems and our poor GC can barely keep up. We were able to secure a starter grant from the Petroleum Research Fund

(administered by the American Chemical Society) in support of our work. Daniel Everson garnered an honorable mention in the NSF Graduate Research Fellowship Program and Ruja Shrestha was chosen to attend the NSF-sponsored CENTC (Center for Enabling New Technologies Through Catalysis) summer school at the University of Washington. Daniel Weix taught CHM 435 Organic Reactions in the fall and found it to be demanding but rewarding. Daniel also helped out with the graduate student recruiting this year (yielding a record number of first-year graduate students anticipated to join the Department this fall) and became a member of the Chemistry Department safety committee. The Weix family, Dan's wife and two children, have acclimated well to their first year in Rochester and Dan looks forward to the coming academic year at the University of Rochester. Includes publications accepted between July 2008 and June 2009.

ROBERT K. BOECKMAN, JR.

1,7,7-Trimethyl-2-azabicyclo[2.2.1]-heptan-3-one. R. K. Boeckman, Jr. and C. G. Collison, *E-Eros*, **2008**, John Wiley & Sons, Chichester, UK.

KARA L. BREN

The Chemistry and Biochemistry of Heme *c*: Functional Bases for Covalent Attachment. S. E. J. Bowman and K. L. Bren, *Nat. Prod. Rep.* **2008**, *25*, 1118-1130.

Modulation of the Ligand-field Anisotropy in a Series of Ferric Low Spin Cytochrome *c* Mutants Derived from *Pseudomonas aeruginosa* Cytochrome *c*-551 and *Nitrosomonas europaea* Cytochrome *c*-552. An EPR and NMR Study. G. Zoppellaro, E. Harbitz, R. Kaur, A. A. Ensign, K. L. Bren, and K. K. Andersson, *J. Am. Chem. Soc.* **2008**, *130*, 15348-15360.

Studies of Ferric Heme Proteins with Highly Anisotropic/Highly Axial Low Spin (S = 1/2) Electron Paramagnetic Resonance Signals with Two Histidines or Histidine and Methionine Axial Fe Coordination. G. Zoppellaro, K. L. Bren, A. A. Ensign, E. Harbitz, R. Kaur, H.–P. Hersleth, U. Ryde, L. Hederstedt, and K. K. Andersson, *Biopolymers* **2009**, *in press.* doi:10.1002/bip.21267

ESTHER M. CONWELL

Spotlight on "Charge Migration along the DNA Duplex: Hole vs. Electron Transport." B. Elias, F. Shao and J. K. Barton, *J. Am. Chem. Soc.* **2008**, *130*, 1152, E. M. Conwell, published in *J. Am. Chem. Soc.* Select Issue 4.

JOSEPH P. DINNOCENZO

An Experimental and Theoretical Study of Triplet Energy Transfer and Electron Transfer in Rigid Polymer Films. P. B. Merkel and J. P. Dinnocenzo, *J. Phys. Chem. A* **2008**, *112*, 10790-10800. Bonded Exciplex Formation: Electronic and Stereoelectronic Effects. Y. Wang, O. Haze, J. P. Dinnocenzo, S. Farid, R. S. Farid, and I. R. Gould, *J. Phys. Chem. A* **2008**, *112*, 13088-13094.

Low-Power Green-to-Blue and Blue-to-UV Upconversion in Rigid Polymer Films. P. B. Merkel, and J. P. Dinnocenzo, *J. Lumin.* **2009**, *129*, 303-306.

Accurate Oxidation Potentials of Benzene and Biphenyl Derivatives via Electron Transfer Equilibria and Transient Kinetics. P. B. Merkel, P. Luo, J. P. Dinnocenzo, and S. Farid, *J. Org. Chem.* **2009**, *74*, 5163-5173.

RICHARD EISENBERG

Synthesis, Electrochemistry, Photophysics and Solvatochromism in New Cyclometalated 6-Phenyl-4-(p-R-phenyl)-2,2'-bipyridyl (R = CH₃, COOCH₃, P(O)(OEt)₂) (C^N^N) Platinum(II) Thiophenolate Chromophores. J. Schneider, P. Du, X. Wayn, W. W. Brennessel, and R. Eisenberg, *Inorg. Chem.* **2009**, *48*, 1498-1506.

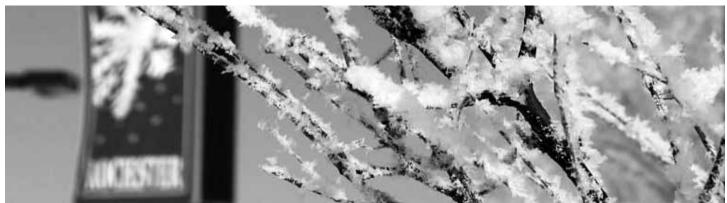
Platinum(II) Terpyridyl-Acetylide Dyads and Triads with Nitrophenyl Acceptors via a Convenient Synthesis of a Boronated Phenylterpyridine. P. Jarosz, K. Lotito, J. Schneider, D. Kumaresan, R. Schmehl, and R. Eisenberg, *Inorg. Chem.* **2009**, *48*, 2420-2428.

Rethinking Water Splitting. R. Eisenberg, *Science* **2009**, *324*, 44-45.

Cyclometalated 6-Phenyl-2,2'-bipyridyl (CNN) Platinum(II) Acetylide Complexes: Structure, Electrochemistry, Photophysics, and Oxidative Reductive Quenching Studies. J. Schneider, P. Du, P. Jarosz, T. Lazarides, X. Wang, W. W. Brennessel, and R. Eisenberg, *Inorg. Chem.* **2009**, *48*, 4306-4316.

Visible Light-Driven Hydrogen Production from Water Catalyzed by Molecular Cobaloxime Catalysts. P. Du, J. Schneider, G. Luo, W. W. Brennessel, and R. Eisenberg, *Inorg. Chem.* **2009**, *48*, 4952–4962.

Snowflakes in Rochester



SAMIR FARID

Bonded Exciplex Formation: Electronic and Stereoelectronic. Y. Wang, O. Haze, J. P. Dinnocenzo, S. Farid, R. S. Farid, and I. R. Gould, *J. Phys. Chem. A* **2008**, *112*, 13088–13094.

Accurate Oxidation Potentials of Benzene and Biphenyl Derivatives via Electron Transfer Equilibria and Transient Kinetics. P. B. Merkel, P. Luo, J. P. Dinnocenzo, and S. Farid, *J. Org. Chem.* **2009**, *74*, 5163-5173.

JAMES M. FARRAR

Singlet and Triplet State Dynamics of Charge and Hydride Transfer Reactions of OD⁺ with Propyne. L. Liu, Y. Li, and J. M. Farrar, *Int. J. Mass Spectrom.* **2009**, *280*, 154.

RUDI FASAN

Evolutionary History of a Specialized P450 Propane Monooxygenase. R. Fasan, Y. T. Meharenna, C. D. Snow, T. L. Poulos, and F. H. Arnold, *J. Mol. Biol.* **2008**, *383*, 1069-1080.

Chemo-enzymatic Fluorination of Unactivated Organic Compounds. A. Rentmeister, F. H. Arnold, and R. Fasan, *Nat. Chem. Biol.* **2009**, *5*, 26-28.

ALISON J. FRONTIER

Origins of Stereoselectivity in the Oxido-Alkylidenation of Alkynes. D. P. Canterbury, A. J. Frontier, J. Um, P. Cheong, D. Goldfeld, R. Huhn, and K. N. Houk, *Org. Lett.* **2008**, *10*, 4597-4600.

Nazarov Cyclization Initiated by Peracid Oxidation: The Total Synthesis of (±)-Rocaglamide. J. M. Malona, K. Cariou, and A. J. Frontier, *J. Am. Chem. Soc.* **2009**, *131*, 7560–7561.

Formal Synthesis of Roseophilin. A. Y. Bitar and A. J. Frontier, *Org. Lett.* **2009**, *11*, 49-52.

A Torquoselective Extrusion of Isoxazoline N-Oxides. Application to the Synthesis of Aryl Vinyl and Divinyl Ketones for Nazarov Cyclization. D. P. Canterbury, J. Um, K. N. Houk, and A. J. Frontier, *Tetrahedron* **2009**, *65*, 3165-3179. (Invited article for Tetrahedron *Symposium-In-Print;* honoring [award winner] Justin DuBois).

PATRICK L. HOLLAND

Electronic Structure and Reactivity of Three-Coordinate Iron Complexes. P. L. Holland, *Acc. Chem. Res.* **2008**, *41*, 905-914.

Mössbauer, EPR, and Theoretical Study of a High-spin, Fourcoordinate Fe(II) Diketiminate Complex. S. Stoian, J. M. Smith, P. L. Holland, E. Münck, and E. L. Bominaar, *Inorg. Chem.* 2008, 47, 8687-8695.

Solid State and Proton NMR Characterization of an Iron(II) Complex of a Tridentate, Facially Coordinating N,N,O Donor Ligand. S. S. Rocks, W. W. Brennessel, T. E. Machonkin, and P. L. Holland, *Inorg. Chim. Acta* **2009**, *362*, 1387-1390.

"Nitrogen Fixation" in McGraw-Hill Yearbook of Science & Technology, P. L. Holland, McGraw-Hill, New York, **2009**, pp. 255-256.

Catalytic Nitrene Transfer from an Imidoiron(III) Complex to Form Carbodiimides and Isocyanates. R. E. Cowley, N. A. Eckert, J. E. Elhaïk, and P. L. Holland, *Chem. Commun.* **2009**, 1760-1762.

Bis(η²-pentamethylcyclopentadienyl)cobalt(II). M. M. Clark, W. W. Brennessel, and P. L. Holland, *Acta Cryst. E* **2009**, *65*, m391.

A Diketiminate-bound Diiron Complex with a Bridging Carbonate Ligand. A. R. Sadique, W. W. Brennessel, and P. L. Holland, *Acta Cryst. C* **2009**, *65*, m174-m176.

Iron(II) Complexes with Redox-Active Tetrazene (RNNNR) Ligands. R. E. Cowley, E. Bill, F. Neese, W. W. Brennessel, and P. L. Holland, *Inorg. Chem.* **2009**, *48*, 4828-4836.

Ligand Dependence of Binding to Three-Coordinate Fe(II) Complexes. K. P. Chiang, P. M. Barrett, F. Ding, J. M. Smith, S. Kingsley, W. W. Brennessel, M. M. Clark, R. J. Lachicotte, and P. L. Holland, *Inorg. Chem.* **2009**, *48*, 5106-5116.

New Routes to Low-Coordinate Iron Hydride Complexes: The Binuclear Oxidative Addition of H₂. T. R. Dugan and P. L. Holland, *J. Organomet. Chem.* **2009**, *694*, 2825-2830. (Special issue on Organometallics for Energy Conversion).

WILLIAM D. JONES

Oxidative Addition of the C–S Bond of Thiophene to the $(C_5Me_5)Rh(PMe_3)$ Fragment: A Theoretical Study Revisited. T. A. Ateşin and W. D. Jones, *Organometallics* **2008**, *27*, 3666-3670.

Experimental and Theoretical Examination of C–CN Bond Activation of Benzonitrile using Zerovalent Nickel. T. A. Ateşin, T. Li, S. Lachaize, J. J. García, and W. D. Jones, *Organometallics* **2008**, *27*, 3811-3817.

An Efficient Low Temperature Route to Polycyclic Isoquinoline Salt Synthesis via C-H Activation with $[Cp^*MCl_2]_2$ (M = Rh, Ir). L. Li, W. W. Brennessel, and W. D. Jones, *J. Am. Chem. Soc.* **2008**, *130*, 12414-12424.

Selectivity in the Oxidative Addition of C-S Bonds of Substituted Thiophenes to the $(C_5Me_5)Rh(PMe_3)$ Fragment: A Comparison

of Theory with Experiment. T. Atesin and W. D. Jones, *Inorg. Chem.* **2008**, *47*, 10889–10894.

Mechanistic Insights on the Hydrodesulfurization of Biphenyl-2-Thiol with Nickel Compounds. J. Torres-Nieto, W. W. Brennessel, W. D. Jones, and J. J. García, *J. Am. Chem. Soc.* **2009**, *131*, 4120–4126.

Selective C–H Activation of Haloalkanes using a Rhodiumtrispyrazolylborate Complex. A. J. Vetter, R. D. Rieth, W. W. Brennessel, and W. D. Jones, *J. Am. Chem. Soc.* **2009**, *131*, 10742–10752.

Synthesis, Characterization, and C–H/C–C Cleavage Reactions of Two Rhodium-Trispyrazolylborate Dihydrides. D. D. Wick and W. D. Jones, *Inorg. Chim. Acta*, **2009**, ASAP. doi:10.1016/j. ica.**2009**.03.022

C-H Activation of Phenyl Imines and 2-Phenylpyridines with $[Cp^*MCl_2]_2$ (M) Ir, Rh: Regioselectivity, Kinetics, and Mechanism. L. Li, W. W. Brennessel, and W. D. Jones, *Organometallics* **2009**, *28*, 3492–3500.

Carbon-Sulfur Bond Cleavage of Methyl Substituted Thiophenes with Iridium(III). M. R. Grochowski, W. W. Brennessel, and W. D. Jones, *Organometallics* **2009**, *28*, 2661–2667.

Unusual Lithium Coordinated Platinum Hydride Dimer and Its Facile Reaction with 2-Cyanothiophene. T. A. Ateşin, W. W. Brennessel, and W. D. Jones, *Inorg. Chim. Acta* **2009**, ASAP. doi:10.1016/j.ica.2009.05.013

JACK A. KAMPMEIER

"Peer-Led Team Learning; Organic Chemistry." J. A. Kampmeier and P. Varma-Nelson in *Chemists' Guide to Effective Teaching Vol. II.* N. Pienta, M. M. Cooper, T. Greenbowe, Eds. (Prentice Hall, Inc. Upper Saddle, NJ) **2008**.

Pedagogies of Engagement in Science: A Comparison of PBL, POGIL and PLTL. T. Eberlein, J. A. Kampmeier, V. Minderhout, R. S. Moog, T. Platt, P. Varma-Nelson, *Biochem. Mol. Biol. Ed.*, **2008**, *36*, 262-273.

TODD D. KRAUSS

Ultra-bright PbSe Magic Sized Clusters. C. M. Evans, L. Guo, J. J. Peterson, S. Maccagnano, and T. D. Krauss, *Nano Lett.* **2008**, *8*, 2896-2899.

A Comparison of Quality of Dispersion of Single Wall Carbon Nanotubes using Different Surfactants and Biomolecules. R. Haggenmueller, S. S. Rahatekar, J. A. Fagan, J. Chun, M. L. Becker, R. R. Naik, T. Krauss, L. Carlson, J. Kadla, P. Trulove, D. Fox, Z. Fang, S. Kelley, and J. W. Gilman, *Langmuir* **2008**, *24*, 5070–5078. Multilayer Film Preparation of PVPh from Aqueous Media. R. Priefer, K. E. Leach, T. D. Krauss, J. R. Drapo, M. L. Ingalsbe, M. A. van Dongen, J. C. Cadwalader, M. A. Baumler, and M. S. Pinto, *Surf. Coat. Technol.* **2008**, *202*, 6109-6112.

Fluorescence from Isolated Carbon Nanotubes in Cross-linked Micelles. K. E. Leach, H. N. Pedrosa, L. J. Carlson, and T. D. Krauss, *Chem. Mater.* **2009**, *21*, 436-438.

Organic Photonic Bandgap Microcavities Doped with Semiconductor Nanocrystals for Room-temperature Single Photon Sources on Demand. S. G. Lukishova, L. J. Bissell, V. M. Menon, N. Valappil, M. A. Hahn, C. M. Evans, B. Zimmermanm T. D. Krauss, C. R. Stroud, Jr., and R. W. Boyd, *J. Mod. Opt.* **2009**, *56*, 167-174.

Biosensors: Nanotubes Light up Cells. T. D. Krauss, Nat. Nanotech. 2009, 4, 85-86.

Non-blinking Semiconductor Nanocrystals. X. Wang, X. Ren, K. Kahen, M. A. Hahn, M. Rajeswaran, S. Maccagnano-Zacher, J. Silcox, G. E. Cragg, Al. L. Efros, and T. D. Krauss, *Nature* **2009**, *459*, 686-689.

"Detection of Methicillin-resistant *Staphylococcus Aureus* (MRSA) using the NanoLantern[™] Biosensor," in Frontiers in Pathogen Detection: From Nanosensors to Systems. C. M. Strohsahl, B. L. Miller, and Todd D. Krauss, Ed: P. M. Fauchet, *Proc. SPIE* **2009**, *7167*, 1-13.

BRADLEY L. NILSSON

The Effect of Increasing Hydrophobicity on the Self-Assembly of Amphipathic Beta-Sheet Peptides. C. J. Bowerman, D. M. Ryan, D. A. Nissan, and B. L. Nilsson, *Mol. BioSyst.* **2009**, *5*, 1058-1069.

LEWIS J. ROTHBERG

Luminescence quenching by charge carriers in organic lightemitting diodes, M. Wyman, A. Marchetti, L. J. Rothberg, R. H. Young, and D. Y. Kondakov, *Digest of Technical Papers - Society for Information Display International Symposium* **2009**, *40*, 306-309.

Plasmon Enhancement of Bulk Heterojunction Organic Photovoltaic Devices by Electrode Modification. X. Chen, C. Zhao, L. J. Rothberg, and M.-K Ng, *Appl. Phys. Lett.* **2008**, *93*, 123302.

Regulation of Electronic Behavior via Confinement of PPVbased Oligomers on Peptide Scaffolds. O. Y. Kas, M. B. Charati, L. J. Rothberg, M. E. Galvin, and K. L. Kiick, *J. Mater. Chem.* **2008**, *18*, 3847–3854. Emissive Efficiency Enhancement of Alq₃ and Prospects for Plasmon-enhanced Organic Electroluminescence. W. Li, S. Pan, and L. J. Rothberg, *Proc. SPIE* **2008**, *7032*, 703224.

W. UDO SCHRÖDER

Effects of H_2O and H_2O_2 on Thermal Desorption of Tritium from Stainless Steel. M. J. Quinlan, W. T. Smayda, S. Lim, S. Salnikov, Z. Chambers, E. Pollock, and W. U. Schröder, *Fusion Science and Technology* **2008**, *54*, 519.

A Simple Method for Rise-Time Discrimination of Slow Pulses from Charge-Sensitive Preamplifiers. J. Tõke, M. J. Quinlan, W. Gawlikowicz, and W. U. Schröder, Report UR-NCUR 06-16.2, *Nuclear Instr. Meth. Phys. Res.* **2008**, *A595*, 460.

Gentle Multifragmentation–a Generalized Fission. J. Tõke and W. U. Schröder, Invited Paper, Proc. Intern. Workshop Multifragmentation and Related Topics, *Soc. It. Fisica* **2008**, *95*, 39-46.

Isoscaling in Statistical Fragment Emission in an Extended Fermi Gas Model. W. Ye, J. Tõke, and W. U. Schröder, *Phys. Lett. B* **2009**, *676*, 193–198.

HARRY STERN

"Coarse-grained and Multiscale Models of Lipid Bilayers," in Multiscale Modeling of Particle Interactions: Applications in Biology and Nanotechnology. H. A. Stern, D. J. Gee and M. R. King, Eds. (Wiley, Hobeken, NJ) **2009**.

Effects of Restrained Sampling Space and Nonplanar Amino Groups on Free-energy Predictions for RNA with Imino and Sheared Tandem GA Base Pairs Flanked by GC, CG, iGiC, or iCiG Base Pairs. I. Yildirim, H. A. Stern, J. Sponer, N. Spackova, and D. H. Turner, *J. Chem. Theory, Comput.* **2009**, *5*, 2088-2100.

Evaluating Docking Methods for Prediction of Binding Affinities of Small Molecules to the G Protein $\beta\gamma$ Subunits. M.-S. Park, A. L. Dessal, A. V. Smrcka, and H. A. Stern, *J. Chem. Inf. Model* **2009**, *49*, 437.

CHING W. TANG

Current Efficiency in Organic Light-emitting Diodes with a Hole-injection Layer. H. Wang, K. Klubek, and C. W. Tang, *Appl. Phys. Lett.* **2008**, *93*, 093306.

DOUGLAS H. TURNER

NMR-Assisted Prediction of RNA Secondary Structure: Identification of a Probable Pseudoknot in the Coding Region of an R2 Retrotransposon. J. M. Hart, S. D. Kennedy, D. H. Mathews, and D. H. Turner, *J. Am. Chem. Soc.* **2008**, *130*, 10233-10239.



The Memorial Art Gallery

Contributions of Stacking, Preorganization, and Hydrogen Bonding to the Thermodynamic Stability of Duplexes between RNA and 2'-O-methyl RNA with Locked Nucleic Acids (LNA). E. Kierzek, A. Pasternak, K. Pasternak, Z. Gdaniec, I. Yildirim, D. Turner, and R. Kierzek, *Biochemistry* **2009**, *48*, 4377-4387.

A CA+ Pair Adjacent to a Sheared GA or AA Pair Stabilizes Size-Symmetric RNA Internal Loops. G. Chen, S. D. Kennedy, and D. H. Turner, *Biochemistry* **2009**, *48*, 5738-5752.

Secondary Structures for 5' Regions of R2 Retrotransposon RNAs Reveal a Novel Conserved Pseudoknot and Regions that Evolve under Different Constraints. E. Kierzek, S. M. Christensen. T. H. Eickbush, R. Kierzek, D. H. Turner, and W. N. Moss, *J. Mol. Biol.* **2009**, *390*, 428-442.

Effects of Restrained Sampling Space and Non-planar Amino Groups on Free Energy Predictions for RNA with Imino and Sheared Tandem GA Base Pairs Flanked by GC, CG, iGiC or iCiG Base Pairs. I. Yildirim, H. Stern, J. Sponer, N. Spackova, and D. H. Turner, *J. Chem. Theory Comput.* **2009**, *5*, 2088-2100.

Bachelors and Masters Degrees Awarded in Chemistry

2009 BACHELOR OF SCIENCE

Ariel Brown Kyle Bulicz Nadia Byrnes Jessica Chery Victoria Chu² Josh Epstein¹ Eric Glowacki² Allison Hulchanski² Colleen Kellenberger^{3†} Ayesha Khan² Katherine Lai Carol Li Matthew Merriman³ Eric Miller^{*} Rebecca Murphy² Eve Privman¹ Matthew Sharpe Ferdous Zannat³ Emily Zbesko

2009 BACHELOR OF ARTS

Vishal Anugu² Mina Ayyad John Bertola^{2†} Evan Bilheimer² Christine Chan Jonathan Chester^{**} Kristen Fitzgerald Elizabeth Lim Daniel Nassau^{1*} John Oakford^{1**} Brian Palmisano^{3†} Tyler Reid Ruth Scoles Alexander Stwertka Alisa Thavikulwat^{3†} Jason Wang Neal Weisbrod^{3†} Sornanong Yaibuathes¹

2009 MASTER OF SCIENCE

George Arab Wesley Asher Charles Bowerman Mehmet Can Jennifer Ciesielski Meghan Clark Ryan Daly Eric DeCoste Todd Doran Stephanie Harding Jesse Kleingardner

Saing Min Lee Pu Luo James Morris Leslie Ofori Brian Ohman Tawana Robinson Derek Ryan Ruja Shrestha Eric Theiste Tulaza Vaidya Hsiu-Ying Wei

DISTINCTIONS

¹Distinction ²High Distinction ³Highest Distinction [†]Phi Beta Kappa *Take 5 Scholar (finishing) **Take 5 Scholar (beginning) *Kauffman Entrepreneurial Fifth Year (KEY) Student

Class of 2009 Bachelor's Degree recipients





The University of Rochester Mace

Doctoral Degrees Awarded in Chemistry

Pingwu Du

Platinum(II) Polypyridyl Complexes for Visible Lightdriven Hydrogen Production from Water Richard Eisenberg Postdoctoral Fellowship, Massachusetts Institute of Technology

Paul Jarosz

Platinum Terpyridine Acetylide Complexes for Photoinduced Charge Separation and the Photogeneration of Hydrogen from Aqueous Media Richard Eisenberg Postdoctoral Fellowship, Rochester Institute of Technology

Kathryn Leach

Carbon Nanotube Optoelectronics Todd D. Krauss Research Scientist, Advanced Concepts and Technologies International

Ling Li

Transition Metal Mediated Synthesis of Heterocycles via Carbon-Hydrogen Bond Activation William D. Jones Postdoctoral Fellow, Columbia University

John Malona

The Catalytic Nazarov Cyclization of Heteroaromatic Systems and its Application Towards Rocaglamide Alison J. Frontier Postdoctoral Fellow, Princeton University

Jacob Schneider

I) Structural and Luminescence Properties of Gold(I) Benzimidazolethiolate Complexes. II) Cyclometalated Platinum(II) Coordination Compounds as Potential Chromophores for the Photogeneration of Hydrogen from Water
Richard Eisenberg
Postdoctoral Fellow, University of York, United Kingdom

Robert Spitale

Chemical and Structural Analysis of RNA-Based Gene Regulation Joseph Wedekind Postdoctoral Fellow, Stanford University

Venkatesan Srinivasan

Studies Directed Toward the Total Synthesis of (-)-Apoptolidin A Robert K. Boeckman, Jr. Postdoctoral Fellow, Scripps Research Institute

Student Awards

DEPARTMENT AWARDS

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

John McCreary Memorial Prize Rebecca Murphy

ACS Rochester Section Award Allison Hulchanski

Merck Index Award Ferdous Zannat

Distinguished Service Award John Bertola

Chemistry Department Award Ayesha Khan Matthew Merriman Brian Palmisano Neal Weisbrod

ENDOWED DEPARTMENT FELLOWSHIPS

Robert and Marian Flaherty DeRight Fellowship

John Miller Walter Moss Michael Quinlan

Arnold Weissberger Fellowship

Abdallah Bitar Pingwu Du Cen Gao Chao Jiang Ling Li Ting Li

Hugh Alan Ewart Fellowship

Lisa Carlson Amy Ensign Samuel Allen and Ellen Frances Lattimore Fellowship Ruja Shrestha Tulaza Vaidya

Elon Huntington Hooker Fellowship Sarah Bowman Amy Ensign Robert Spitale

COLLEGE AWARDS

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

Ayman-Amin Salem Award Colleen Kellenberger

Catherine Block Memorial Fund Prize Julie Tabroff

TEACHING AWARDS

W. D. Walters Teaching Award John DiMaio Todd Doran James Morris

Carl A. Whiteman Jr. Teaching Award Kyle Bulicz Ananya Ray

Distinguished Teaching Award Neal Weisbrod

PHI BETA KAPPA

John Bertola '09, Colleen Kellenberger '09, Brian Palmisano '09, Alisa Thavikulwat '09, Neal Weisbrod '09

Fellows '08-'09

Elizabeth Anderson State University of New York at Stony Brook

Zhihui Ban University of New Orleans; Zhejiang Univ., P.R. China

Kevin Cariou Université Pierre et Marie Curie, Paris, France

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

Benjamin Dible University of Utah, Salt Lake City, UT

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

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

Theodore Lazaridis University of Sheffield, UK; Aristotle University of Thessaloniki, Greece

Andrea Lee University of Wisconsin-Madison, Madison, WI

Matthew Liptak University of Wisconsin-Madison, Madison, WI

Genggeng Luo Xiamen University, Xiamen, P.R. China

Theresa McCormick Queen's University, Kingston, Ontario, Canada

Alexey Novikov Technische Universität Chemnitz, Chemnitz, Germany

Hardey Singh Panjab University, Chandigarh, India Taro Tanabe Institute for Chemical Research, Kyoto University, Kyoto, Japan

Xiaoyong Wang University of Arkansas, Fayetteville, AR

Ilyas Yildirim University of Rochester- Physics, Turkey

Jing Zhang Nanjing University, P.R. China

The University Seal on a medal



Seminars & Colloquia

JULY 2008

Sarah Bowman (University of Rochester) "NMR Studies of the Iron-histidine Interaction in Paramagnetic Cytochromes c," July 14, 2008.

Julie Smyder (University of Rochester) "Progress Toward Simultaneous Charge and Fluorescence Measurements," July 18, 2008.

Paul R. Jarosz (University of Rochester) "Platinum Terpyridine Acetylide Complexes for Photo-Induced Charge Separation and the Photogeneration of Hydrogen from Aqueous Media," July 31, 2008.

AUGUST 2008

Joaquin Calcines (University of Rochester) "Oriented Attachment Growth Mechanism for Cadmium Selenide Nanorods," August 12, 2008.

Ilyas Yildirim (University of Rochester) "Free Energy Calculations of RNA Duplexes with Tandem GA Base Pairs using the Thermodynamic Integration Approach," August 12, 2008.

SEPTEMBER 2008

James Kovach (University of Rochester) "*Transition Metal Silylene Complexes*," September 8, 2008.

Professor Yoshihisa Kobayashi (University of California at San Diego) *"Heterocycles in Natural Product Synthesis,"* September 12, 2008.

Professor David Watson (SUNY Buffalo) "Photoinduced Electron Transfer Processes of Self-Assembled Inorganic Nanomaterials," September 15, 2008.

SEYMOUR ROTHCHILD LECTURE

Professor Brian Hoffman (Northwestern University) *"Towards the Mechanism of* N_2 *Reduction by Nitrogenase,"* September 17, 2008.

Dr. Louis N. Jungheim (Lilly Corporate Center) *"New Twists in Nazarov Cyclization Chemistry,*" September 17, 2008.

John Malona (University of Rochester) "The Catalytic Nazarov Cyclization of Heteroaromatic Systems and its Application Towards Rocaglamide," September 19, 2008.

Professor Jeremy M. Smith (New Mexico State University) "One and Two Electron Transformations of High Valent Iron Imido and Nitrido Complexes," September 22, 2008.

Professor Vladimir Gevorgyan (University of Illinois at Chicago) "*Development of Novel Transition Metal-Catalyzed Synthetic Methodologies*," September 24, 2008.

Professor Rory Waterman (University of Vermont) "*Zirconium-catalyzed Bond-forming Reactions*," September 28, 2008.

OCTOBER 2008

Professor Yan-Yeung Luk (Syracuse University) "Principles for Amphiphile-Free Water-in-Water Emulsions: Templated Synthesis and Biocatalysis," October 3, 2008.

Professor Michael Jennings (The University of Alabama) "Total Syntheses of β -C-Glycoside Natural Products via Oxocarbenium Cations," October 10, 2008.

INAUGURAL MAGOMEDOV-SHCHERBININA MEMORIAL PRIZE AND LECTURESHIP

Professor Sergey A. Kozmin (University of Chicago)

"Practical Organic Synthesis to Unravel Chemical Biology of Complex Natural Products," October 15, 2008.

ANDREW S. KENDE DISTINGUISHED LECTURE

Professor Brian M. Stoltz (California Institute of Technology)

- *I. "Complex Natural Products as a Driving Force for Discovery in Organic Chemistry,"* October 21, 2008.
- II. "Oxidation Catalysis: The Development of Aerobic Based Oxidation Methodology for Synthetic Chemists," October 22, 2008.
- III. "The Intertwined Nature of Chemical Synthesis and the Discovery Process," October 23, 2008.

Professor Peng Chen (Cornell University) "Single-Molecule Dynamics of Bioinorganic Chemistry and Nanocatalysis," October 27, 2008.

Professor Robert Hondal (University of Vermont) "Selenium in Thioredoxin Reductase: A Mechanistic Perspective," October 31, 2008.

NOVEMBER 2008

Professor John Golbeck (Pennsylvania State University) *"A Hybrid Biochemical/Organic Half-Cell for the Photochemical Generation of Dihydrogen,"* November 5, 2008.

Professor Joel Schneider (University of Delaware) "*Peptide-based Materials*," November 7, 2008.

W. ALBERT NOYES, JR. MEMORIAL LECTURE

Professor James L. Skinner (University of Wisconsin)

- I. "Water: Hydrogen Bonding in the Bulk Liquid and at the Liquid/vapor Interface, and New Simulation Models," November 10, 2008
- II. "Water: Traditional, Ultrafast and Sum-frequency Vibrational Spectroscopy of the Bulk Liquid and the Liquid/ vapor Interface," November 11, 2008.
- III. "Membrane Peptides: 2D-IR Spectroscopy as a Probe of Structure and Dynamics," November 12, 2008.

Professor Guy Lloyd-Jones (The Bristol Centre for Organometallic Catalysis) *"Mechanistic Studies of Pd-catalyzed Allylic Alkylation: Simple, Subtle and Complex,"* November 24, 2008.

DECEMBER 2008

Professor Felix N. Castellano (Bowling Green State University) *"Molecular Inorganic Photonics,"* December 3, 2008.

Dr. Louise Berben (Massachusetts Institute of Technology and California Institute of Technology) *"Chemistry and Electrochemistry with Small Molecules at First Row Transition Metal Centers,"* December 4, 2008.

Professor Wilfred van der Donk (University of Illinois) "Biosynthesis of Lantibiotics, Polycyclic Thioether Antibiotics," December 5, 2008.

Dr. Aihua Fu (Stanford University) "Lighting up New Functionalities of Nanoparticles," December 8, 2008.

Dr. Khalid Salaita (University of California, Berkeley) "Deconstructing Receptor Signaling with Chemically Tailored Interfaces," December 11, 2008.

Dr. Dwight Seferos (Northwestern University) "Conjugated Oligomers and Polyvalent Nanoparticle Conjugates," December 18, 2008.

Venkatesan Srinivasan (University of Rochester) "Studies Directed Toward the Total Synthesis of (-)-Apoptolidin A," December 19, 2008.

JANUARY 2009

Dr. Samuel W. Thomas, III (Harvard University) *"New Functions of Organic Materials,"* January 5, 2009.

Dr. Yuan-Chung Cheng (University of California, Berkeley) "Theory of Excitation Energy Transfer and Threepulse Photon-echo Spectroscopy with Applications to Photosynthetic Pigment-protein Complexes," January 8, 2009. Dr. Eric Strieter (Harvard University) "Non-Canonical Assembly-Line Biosynthesis: The Story of Coronatine Biogenesis," January 15, 2009.

FEBRUARY 2009

Professor Joseph A. Schmidt (The University of Toledo) *"Catalytic Coupling Reactions using Hemilabile Phosphino-Imines and Palladium,"* February 20, 2009.

HUTCHISON MEMORIAL LECTURE

Professor Michael R. Wasielewski (Northwestern University)

- I. "Energy and Charge Transport in Self-assembled Systems for Solar Energy Conversion," February 24, 2009.
- II. "Dynamics of Photogenerated Multi-Spin Systems: The Road to Molecular Spintronics," February 25, 2009.
- III. "Molecules as Wires: Structural and Electronic Criteria for Long Distance Charge Transport," February 26, 2009.

MARCH 2009

Professor Song Jin (University of Wisconsin-Madison) *"How to Make Nanowire Christmas Trees: Screw Dislocation Driven Nanowire Growth,*" March 2, 2009.

Professor Kay Brummond (University of Pittsburgh) *"Exploiting Under-Utilized Functional Groups in Chemical Reaction Discovery and Library Synthesis,"* March 4, 2009.

Professor Ann M. Valentine (Yale University) "Bioinorganic Chemistry of Titanium in Medicine and the Environment," March 16, 2009.

Professor Benoit Roux (University of Chicago) "Multiscale Approach to the Activation/Inactivation of Src Kinases," March 18, 2009.

Pu Luo (University of Rochester) "Mechanism for the Lewis Acid Catalyzed Cycloadditions of Aldehydes and Donor-Acceptor Cyclopropanes," March 20, 2009.

Professor Brent Gunnoe (University of Virginia) "Development of Homogeneous Catalysts for the Conversion of C-H Bonds," March 30, 2009.

APRIL 2009

Professor Julius Rebek (The Scripps Research Institute) *"The Inner Space of Molecules,"* April 1, 2009.

Pingwu Du (University of Rochester) "Platinum (II) Polypyridyl Complexes for Visible Light-driven Hydrogen Production from Water," April 2, 2009.

Professor Jiali Gao (University of Minnesota) "Dynamic Contributions to Enzyme Catalysis as Illustrated by Orotidine Monophosphate Decarboxylase (OMPDC)," April 6, 2009.

Professor Paul Barbara (University of Texas at Austin) "A Single Molecule Spectroscopy Investigation of the Electronic Properties of Conjugated Polymers," April 8, 2009.

Matthew Betush (University of Rochester) "Recent Methodologies Towards Highly Substituted Pyrroles," April 10, 2009.

Matthew McLaughlin (University of Rochester) "Directed Evolution as a Tool for Engineering P450 BM-3 into a Propane Hydrolase," April 13, 2009.

Kathryn Elizabeth Leach (University of Rochester) *"Carbon Nanotube Optoelectronics,"* April 14, 2009.

Robert Spitale (University of Rochester) "Chemical and Structural Analysis of RNA-Based Gene Regulation," April 16, 2009.

Professor Mukund Sibi (North Dakota State University) "Achiral Templates. New and Effective Tools for Asymmetric Transformations," April 17, 2009.

Ling Li (University of Rochester) "Transition Metal Mediated Synthesis of Heterocycles via Carbon-Hydrogen Bond Activation," April 17, 2009.

Professor John Dawson (University of South Carolina) "Mechanistic Studies of Oxidative Halophenol Dehalogenation by Heme-Containing Enzymes," April 22, 2009. Professor Tomislav Rovis (Colorado State University) "Ring-Forming Strategies in Asymmetric Catalysis," April 24, 2009.

Professor Oleg Prezhdo (University of Washington) "Dynamics on the Nanoscale: Time-domain ab initio Studies of Photo-induced Dynamics in Quantum Dots and Carbon Nanotubes," April 27, 2009.

Professor Mark Lautens (University of Toronto) *"Synthesis and Reactions of Heterocycles,"* April 29, 2009.

MAY 2009

Professor Julia Brumaghim (Clemson University) "Developing a Predictive Model for Polyphenol Prevention of DNA Damage," May 4, 2009.

Professor Matthew Sigman (University of Utah) *"Metal-Catalyzed Oxidation Reactions for Organic Synthesis,"* May 8, 2009.

Professor Jeffrey Johnson (University of North Carolina) "Reagent and Reaction Development in Organic Chemistry: Recent Case Studies," May 15, 2009.

Kristina Wilson (University of Rochester)

"Beyond the Harmonic Oscillator Approximation: Probing Vibrational Anharmonicity with Ultrafast Vibrational Spectroscopy," May 26, 2009.

Professor Thomas Lectka (Johns Hopkins University) *"New Studies in Catalytic, Asymmetric Alpha-Fluorination,*" May 29, 2009.

Keying Ding (University of Rochester) "Synthesis and Reactivity of Low-coordinate Cobalt Dinitrogen, Hydride and Fluoride Complexes," May 29, 2009.

JUNE 2009

Professor Sean M. Decatur (Oberlin College)

"Spectroscopic Approaches to Protein AGGREGATION Diseases: Conformation and Dynamics of Amyloid Aggregates via Isotopeedited Infrared Spectroscopy," June 3, 2009.

Nanomaterials Symposium 2009

Professor George Whitesides (Harvard University) "Materials Science, Nanoscience, and Energy," May 11, 2009.

Professor Ching W. Tang (University of Rochester) "Thin-film PhotovoltaicTechnologies--Prospects and Challenges," May 11, 2009.

Professor Philippe Fauchet (University of Rochester) "Nanoscience and Nanostructures for Solar Energy," May 11, 2009.

Professor Louis Brus (Columbia University) *"Carbon Nanotubes and Graphene,"* May 11, 2009.

Professor Hong Yang (University of Rochester) "Design, Synthesis, Formation Mechanism and Electrocatalytic Applications of Platinum and Its Alloy Nanostructures," May 11, 2009.

Professor Matthew Yates (University of Rochester) "Synthesis of Proton Conducting Ceramic Membranes via Seeded Surface Crystallization," May 11, 2009.

Professor Vicki Colvin (Rice University) "Understanding and Applying Nanoparticles in the Environment," May 12, 2009.

Professor Michael Grunze (University of Heidelberg) "Surface Interactions and Reactions in Marine Fouling," May 12, 2009.

Professor Alison Elder (University of Rochester)"Strategies for Testing the Safety of Nanomaterials," May 12, 2009.

Professor James McGrath (University of Rochester) "Porous Nanocrystalline Silicon Membranes for Efficient and Precise Molecular Separations," May 12, 2009.

Professor Ashutosh Chilkoti (Duke University) "Nanostructures of Macromolecules to Direct Biological Function," May 12, 2009.

Professor Benjamin Miller (University of Rochester) "Nanostructured Materials for Optical Biosensing," May 12, 2009.

Professor Darrin M. York (University of Minnesota) *"Molecular Simulations of Ribozyme Catalysis,"* June 3, 2009.

Michael Quinlan (University of Rochester) "Nuclear Energy and the Study of Nuclear Matter Far from Stability," June 15, 2009.

Professor Kei Takeda (Hiroshima University) "Development of New Synthetic Methodology Featuring Tandem-Bond Forming Process and Their Application to the Total Synthesis of Natural Products," June 16, 2009. Abdallah Youssef Bitar (University of Rochester) "Progress toward the Total Synthesis of Roseophilin," June 16, 2009.

Meagan Evans (University of Rochester) "Metal-Initiated Amination of Alkenes and Alkynes," June 19, 2009.

Christopher Evans (University of Rochester) "Rational Synthesis and Reaction Mechanism for Chalcogenide Magic-sized Clusters and Quantum Dots," June 22, 2009.

Distinguished and Special Lectures



NEWS FROM THE ADMINISTRATIVE STAFF:

KENNETH SIMOLO (PH.D. '85) this year celebrates his twenty-first 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. In addition, he oversees the day-to-day operations and budget for the Chemistry Department. While a graduate student at Rochester, Ken earned his doctoral degree under the direction of George L. McLendon.

KAREN S. DEAN is in her fifth year in the Department of Chemistry as Administrative Assistant, where she sees to the needs of the Department Chair, the Chair of the Faculty Recruiting Committee, supervises administrative staff, and manages the employment and immigration requirements for Chemistry's postdoctoral research associates. Karen enjoys all the facets of her work and the camaraderie within the Department. This past year, Karen was one of two recipients of the Sandra Beach Memorial award for outstanding service to the Department. She is a dog lover, owner and new member of a local Labrador Retriever rescue group.

DONNA J. DOLAN is a long time staff member in the Department of Chemistry. She is currently in her twenty-first 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.

DEBRA HARING, Development Administrator for Chemistry, is now in her eighth year in the Department of Chemistry and her tenth at the University of Rochester. Debra's responsibilities include facilitating alumni outreach, coordinating faculty (and student) award nominations, pre-proposal faculty support in grant submissions, editorship of departmental publications such as this Newsletter, as well as assisting with special events for the Department. Last year, those events included the Inaugural Magomedov-Shcherbinina Prize and Lectureship, the annual ACS Alumni Social Hour, Meliora Weekend, and NanoSymposium 2009. A major focus in 2008/09 was the redesign/recoding of the Chemistry website-Chemistry now enjoys a contemporary and interactive Internet site that receives an average 4,000 unique visitors per month. Special thanks to our talented student assistant JOHN BERTOLA (B.A. '09) for all of his creativity and diligence in working on the website! In grant work, Debra provides administrative support, particularly to beginning faculty, and serves as the

administrator for the Graduate Assistance in Areas of National Need (GAANN) program. We are gratified that the Chemistry Department continues to receive significant federal support, including economic stimulus funding, for its research and educational programs. A personal highlight last December was the opportunity to attend the 60th birthday symposium of Shaul Mukamel at UCI. Debra's career in Chemistry began as Prof. Mukamel's assistant and it was wonderful to have the opportunity to visit one of her favorite professors, his family, and many former Mukamel group members from the Rochester days at that special celebration!



Debra Haring and John Bertola (B.A. '09) at the 2009 Chemistry Diploma Ceremony

ROBIN COOLEY, Graduate Studies Coordinator, has now been with the Department for five years working in the Graduate Studies office. 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. In February 2009, Robin organized the Department's main recruitment activity, Visitation Weekend, which drew a large number of prospective graduate students. The weather was unusually balmy that weekend and all attendees had a wonderful time meeting with faculty, touring Chemistry's facilities and socializing with our current graduate students in Rochester. Recruitment efforts were highly successful and Chemistry welcomes an incoming class of thirty-one first-year students for 2009-2010. Robin organizes the busy week of Orientation for these students, held in late August as well as helping to coordinate the graduate fellowship program.

TERRI CLARK is the newest addition to the Chemistry Department staff, having moved to New York from California with her husband, who left private consulting to head up the Property Tax Division at Xerox in August 2008. Terri replaced Kathy Adamski as the Undergraduate Studies Program Coordinator and Course Administrator. She also assists faculty in pre-proposal grant preparation, working closely with Debra Haring. Terri came to the University from a wide range of educational and medical administration experience. With both elementary and secondary teaching credentials, she most recently worked for many years at a private, K-8 grade school in the Bay Area (northern California), first teaching fifth grade and computer applications and then moving into administration as Principal. A key interest was developing educational plans and curriculum for struggling students of all ages. Prior to that, she taught private piano lessons, worked as the administrator of a workers compensation evaluation and rehabilitation clinic, and for a group of emergency physicians who staffed hospital emergency departments across the nation. In between, she and her husband raised four children - the two girls both were married over this past year. Terri enjoys learning new software applications, working on all kinds of projects, and being busy with challenging ventures - which means the Chemistry Department is the perfect fit for this beach and mountain loving transplant!



Terri Clark at the 2009 Chemistry Diploma Ceremony

MARGUERITE WESTON, Assistant to Faculty, has been with the Department of Chemistry for fourteen years. She coordinates the Chemistry Seminar Program and produces the online seminar schedule each month. Marguerite also provides support to numerous faculty members, including coordinating select special events, and assisting with projects and class needs. Marguerite assists Professor Thomas Krugh with the many administrative details of Chemistry's National Science Foundation supported annual summer research program for undergraduates (REU), which attracts approximately 125 applications each year from undergraduates across the nation and the University of Rochester. She also assists Professor Krugh in preparing the NSF competitive renewal proposals for each three-year period as well as the grant's annual and final reports. Last spring the Department was awarded a three-year renewal by NSF for its REU Program and once again, the Chemistry Department's summer REU program took place.

ELLY YORK joined the Chemistry Department in November of 2006. 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 continues to work 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. Last summer Elly completed a Master's degree in education. She is also happy to announce her marriage on April 11, 2009 to Brandon York from Rochester, NY!



Newlyweds Elly and Brandon York, April 2009

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

KIRSTIN CAMPBELL joined the staff of *Inorganic Chemistry* in December 2004 and continues to enjoy her position as Chief Editorial Assistant. Out of 45 journals in their category, Inorganic Chemistry is once again the most-cited journal in inorganic chemistry with a record 68,356 total citations, an increase of 6.5% over 2007 and an impact factor of 4.147 in 2008, its highest ever, up slightly from its previous record 4.123 in 2007. Kirstin continues to spend a considerable amount of time overseeing the upgrades to deployment and development of the web based system and website for the journal. The new system has been in use by all ACS journals since 2007. The Rochester office, the main office of the journal, overseen by Editor-in-Chief Richard Eisenberg, handled over 2,400 manuscripts in 2008 and added its first international office in Hong Kong. Inorganic Chemistry also published two special Forum issues in 2008: a Forum on Making Oxygen in March 2008 and a Forum on Functional Inorganic Materials in October 2008. IC is currently working on two more Forum issues for the remainder of this year: one on Magnetism (to be published in March) and one on Nitric Oxide (publication date yet to be determined). IC is one of the few ACS journals featuring issues with a changing cover, being published twice a month. ARLENE BRISTOL continues to enjoy working parttime as Senior Editorial Assistant. She excels at her hobby of playing duplicate bridge in her spare time. This past winter,

MARCIA EISENBERG joined the editorial office part time, assisting with travel and serves as an administrative assistant to the growing journal office.

VALERIE FITZHUGH has been working as an editorial assistant in the Department of Chemistry for almost eight 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) in December 2002. Interacting with authors, editors and reviewers in this role has been an enriching experience for Val. She enjoys the fast pace of the JACS editorial office, and all aspects of processing the 460+ submitted manuscripts to editorial decision and/or production. Assisting authors of cutting-edge science publish their work has made her career a very satisfying and rewarding one. JACS is the premier, stateof-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. JACS submissions were at 4293 YTD as of June 1, 2009. The 2008 ISI Journal Citation Reports recently reported that the Journal of the American Chemical Society was once again the most-cited journal in chemistry with a record 318,252 total citations, an increase of 7.7% over 2007 and more than twice that of the second-ranked journal in total citations, Angewandte Chemie International Edition, which recorded 139,534 total cites. Additionally, JACS achieved its highest impact factor ever of 8.091 in 2008, up from 7.885 in 2007. It looks like it may be another banner year at JACS.

TERRELL SAMORISKI completed her fifth year as Editorial Assistant for The Journal of Organic Chemistry (JOC) in August 2009. 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 webbased submission procedure, the journal now has expanded for the first time, to include an associate editor's office in Europe. According to the most recent ISI statistics for 2008, JOC remains number one in total citations in organic chemistry, with 86,564 cited for the year 2008, translating to an increase of 1.5% in total citations since 2007. In Rochester in 2008, the editorial office handled more than 250 manuscripts. The journal publishes 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.

DAWN MURPHY completed her first year as an editorial assistant to both the *Journal of Organic Chemistry (JOC)* and *Journal of the American Chemical Society (JACS)*. She continues to enjoy assisting Terrell Samoriski and Valerie Fitzhugh in their respective roles as editorial assistants. Dawn enjoys the diversity

and challenge of working in two different journal offices. 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 has to offer and really appreciates being close to family and friends.



Dawn Murphy, our newest Editorial Assistant

NEWS FROM THE SCIENTIFIC AND TECHNICAL STAFF:

ERIC LOBENSTINE (PH.D. '81) reports that the transition to a new Sun email/web server went smoothly in November. Well, mostly, since he deleted his own email in the process, but he didn't lose anything critical! The new email server allows department members to collect their email more easily when they are away from their offices; web access is more secure as well. Our new web server software provides the tools needed for more dynamic, database-driven websites, and we will be deploying a new web application to facilitate the Faculty application and review process. It has been a pleasure to work with JOHN BERTOLA (B.A. '09), our primary web-designer, who graduated this past May. We will miss his expertise as he continues his Masters at the Warner School! Eric also really appreciates the support of the Department and the other Technical Staff, which allowed him to take a three-week vacation to New Zealand and Hawaii with his family, in celebration of his 25th wedding anniversary.

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 2008-2009, minor renovations of Hutchison Hall 421, B04A and B04 were undertaken: B04 was converted into an

undergraduate CG room, B04A was renovated for a Bruker FTMS, and Hutchison Hall 421 was converted into a user facility for housing a microwave and hydrogenation apparatus. Ray continues to enjoy the daily interactions with faculty and students in addressing research and facilities issues. Football (soccer) continues to play a big part in Ray's spare time despite an ACL injury sustained during a pick-up game.

The X-ray crystallography facility, under the direction of crystallographer BILL BRENNESSEL, has continued to provide the high quality service that is expected of the University of Rochester's Chemistry Department. Undergraduate, graduate, postdoctoral and researchers alike readily submit cutting-edge research samples for evaluation to obtain solidstate confirmation for their new molecules. This form of



characterization is very common in all top level journal publications. While all researchers are interested in the independent proof of compounds, inorganic and organometallic research groups are especially interested in bond lengths and bond angles, as well as three-dimensional packing motifs. Organic research groups often use this technique to determine absolute or relative stereochemistry when results from experiments like NMR are ambiguous. Instrument usage is at an all-time high, and data is often collected over the weekends due to the demand. Each year undergraduate students get hands-on training as part of CHM 234. A graduate level course in X-ray crystallography is taught once a year (CHM 417), in which students learn the theory and run a full experiment from crystal selection to presentation of results. Additionally, students who complete the graduate course become officially trained facility users and can run their own research samples. For the upcoming year Bill plans on maintaining the high quality of service, while increasing the number of outside clients. This past year, Bill was one of the recipients of the Sandra Beach Memorial award for outstanding service.



Chemistry faculty and students are aided in their research by numerous invaluable scientific and technical staff. The Department appreciates the efforts and contributions of senior scientists PAUL (Dinnocenzo MERKEL JAN research group), TÔKE (Schröder research group), scientists WILLIAM DAVID HERKSTROETER, HICKEY (PH.D. '85) and SANDIP SUR, Instructor

BRUCE TODER (POSTDOCTORAL FELLOW '82), Instrument Model Maker **KEN ADAMS** and Senior Lab Engineers, **TED O'CONNELL** and **PETE SERRINO**.

NEWS FROM THE SCIENCE LIBRARY:

SUE CARDINAL, Chemistry Librarian from the Carlson Library reports that the library has added REAXYS, a web version of Beilstein and Gmelin. Susan Gibbons was appointed the new Vice Provost & Dean of the River Campus Libraries. The chemistry serials collection has been carefully reviewed and most print subscriptions will be discontinued in 2010 due to current economic conditions. Fortunately, the electronic versions will continue. Sue was the 2008 Chair of the Chemistry Division of SLA (an international library association). On a more personal note, Sue and her husband are enjoying parenthood and are the proud parents of a baby boy - Torstan Cardinal arrived into this world on September 13, 2008.



Sue Cardinal holding newborn baby Torsten, September 2008

NEWS FROM THE BUSINESS OFFICE:

DORIS WHEELER, Business Office Manager since 2002, is pleased to report that she and her colleagues are working effectively together, with no changes in personnel during the past year. The 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. They have also been busy assisting in administering the GAANN Fellowship funding awarded in 2005. The Business Office staff consists of several members. RANDI SHAW, part-time Chemistry Accounting Bookkeeper is responsible for billing internal charges, purchase orders, reconciling ledgers, travel and conference forms, and processing invoices. DIANE EVANS, Staff Accountant, is responsible for reconciling grant ledgers, P-card management and graduate student payroll, and provides backup for Randi's position. DIANE VISIKO, TAR Accounting Bookkeeper, continues to work with departmental payroll and is the 'Timekeeper' for HRMS. PAUL LIBERATORE continues to provide service as the manager of the chemistry stockroom located in the basement of Hutchison Hall. This year we have two staff members in the Business Office celebrating milestone anniversaries-Diane Evans has been working at UR for 10 years and Randi Shaw for 20 years. Congratulations and thank you for the many years of valued service to the University!

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

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

	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 http://www.chem.rochester.edu/alumni/
Contact I NAME	nformation:	Degree Information: Year degree(s) received from the Department B.A.
ADDRESS		B.S M.S PH.D
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NEWSLETTER COMMENTS		



DID YOU KNOW...

...that Rochester's largest employer is also one of the best places in the nation for scientists to work, according to *The Scientist* magazine? The University was rated among the top 10 nonprofit institutions in the nation in the magazine's annual ranking of "Best Places to Work". Scientists rated the University highly, citing the professionalism and collegiality of their peers. The University also received high marks in the areas of teaching and mentoring.



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

A new fund 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.

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)

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	ADVISOR	

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



DID YOU KNOW ...

...there is an interactive website, created by Professor Alison Frontier, that de-mystifies critical laboratory techniques and experimental skills for students? *Not Voodoo* provides a broad scope of free information including a list of common mistakes, roadmaps describing the anatomy of a reaction, and descriptions of fundamentally important, yet surprisingly difficult operations for the beginning research chemist. Check it out at http://chem.chem.rochester.edu/~nvd/.

