

*Chemistry*

2014-2015

Newsletter





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# Faculty and Staff

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Randi Shaw

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Doris Wheeler

### STOCKROOM

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Kate Reinhardt

Elly York

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Kara L. Bren

Joseph P. Dinnocenzo

Richard Eisenberg

James M. Farrar

Rudi Fasan

Ignacio Franco

Alison J. Frontier

Joshua L. Goodman

Pengfei Huo

William D. Jones, Jr.

Todd D. Krauss

Thomas R. Krugh

Ellen Matson

David W. McCamant

Michael L. Neidig

Bradley L. Nilsson

Lewis J. Rothberg

W. Udo Schröder

Douglas H. Turner

Daniel J. Weix

### INSTRUCTIONAL FACULTY

Benjamin Hafensteiner

David Hickey

Bruce Toder

### PROFESSORS EMERITI

Andrew S. Kende

Robert W. Kreilick

John S. Muenter

William H. Saunders, Jr.

### RESEARCH PROFESSORS

Samir Farid

Ralph Young

### SENIOR SCIENTISTS

William Begley

Sanela Lampa-Pastirk

Alfred Marchetti

Brendan Mort

### CHEMISTRY LIBRARIAN

Sue Cardinal

# From the Chair

Greetings to Chemistry Department students, faculty, staff and especially our alumni! It has been an exciting and eventful year for the Chemistry Department and I am delighted to share with you some of the developments within Chemistry and the University during this past year, my third as Chair of the Department. A strong determinant of the success of the Department is the quality of the faculty, and we were delighted to welcome three extremely talented assistant professors to the Department in the past year: Pengfei (Frank) Huo and Ellen Matson, who started in July of 2015, and Kathryn Knowles, who will join the faculty in July of 2016.



Frank Huo is a theoretical chemist who comes to Rochester after a Ph.D. at Boston University and a Postdoctoral Appointment at the California Institute of Technology. Frank is developing new theoretical methods to study the dynamics of light harvesting and proton coupled electron transfer, which has direct applications to understanding solar fuels photochemistry. Ellen Matson got her Ph.D. at Purdue and pursued postdoctoral research at the University of Illinois at Urbana-Champaign. Ellen's planned research seeks alternative applications of fundamental inorganic building blocks for the formation of first-row transition metal complexes capable of facilitating desirable multi-electron transformations with direct applications to some of the most challenging energy-related problems. Lastly, Katie Knowles is not only joining the faculty but is also an alumnus, having earned a B.S. in Chemistry at Rochester in 2008. She then went on to earn a Ph.D. at Northwestern and is currently finishing up a postdoctoral fellowship appointment at the University of Washington. When she officially returns to Rochester in July of 2016, Katie will be developing new syntheses and characterizing the photophysical properties of novel metal-oxide nanoparticles, as well as studying the excited-state dynamics of nanostructured thin-film metal oxide semiconductor-electrolyte interfaces. We expect to be hearing about great things in the near future from this new trio!

The Chemistry faculty continue to be recognized for their excellence in research, the details of which you will hopefully enjoy reading in this newsletter. In particular, we want to highlight Daniel Weix, who received the Novartis Early Career Award in Organic Chemistry. Also, Michael Neidig had an excellent year, winning an NSF Faculty Early Career Development award and a Sloan Research Fellowship. Finally, I want to make a special note regarding Doug Turner, who after 40 years of service to the Department, decided to retire from full-time teaching in June of 2015. Doug will still be very active in studying the biophysical chemistry of RNA, and will now have the luxury to pursue that activity full-time. Many congratulations to Doug on the next phase of his scientific career!

We are proud of the accomplishments of our students, both undergraduate and graduate, many of whom have received a number of awards this year that are listed on our student awards pages. Our graduate program had quite a busy year as 12 students have received their doctoral degrees since May 2015. The large numbers of students graduating in the last 1.5 years (22) has decreased the total number of graduate students currently enrolled to 89, to go along with 19 postdoctoral fellows. The Department welcomed a class of 19 new Ph.D. students in Fall 2015, and with the likelihood of several new faculty hires coming on

board in the next few years, we are striving to enroll approximately 120 students to form an outstanding chemistry graduate student cohort going forward.

Likewise, our undergraduate program continues to excel at the highest level. This past May, we graduated 33 seniors, and will have close to 50 chemistry majors in the senior and junior classes this coming academic year. Of special note is that for the first time we offered a general chemistry course specifically for Engineering and Physics students. The course, designed and taught by James Farrar, will bring a more comprehensive Chemistry experience for the Engineers, and given the increase in undergraduate Engineering enrollments, will potentially attract over 125 students. Of course, hands-on experiential learning, pioneered by Chemistry faculty such as the late Jack Kampmeier, will be central to the experience of the students in the course.

Last year the College and the Chemistry Department agreed on a framework to expand the faculty size to 24 (from the current 19) over the next 5 to 7 year timeframe. We are still working with the College to turn this commitment into a reality. This expansion in total faculty size I believe is critical to maintaining our core strengths in organic, inorganic, and physical chemistry, while also pursuing faculty whose research interests extend to interdisciplinary fields such as biological or materials chemistry, or the chemistry of energy or nanoscience. However, a major roadblock to quickly increasing faculty size is being able to afford the large initial start-up costs to attract top faculty talent to Rochester. To that end I would like to highlight a relatively new endowed fund, named to honor Rich Eisenberg, the Tracy H. Harris Professor Emeritus of Chemistry. The proceeds from this fund will be used to endow a Chaired Professorship in the general areas of inorganic chemistry and/or photoinduced charge transfer and photocatalysis. Like the Andrew Kende Chair of Organic Chemistry, which reached its monetary goal last year, our goal is to use the Eisenberg Chair to help attract top caliber senior faculty to Rochester while also expanding the faculty size overall. The invaluable support of our alumni in aiding the efforts to expand the faculty are sincerely appreciated and cannot be overstated.

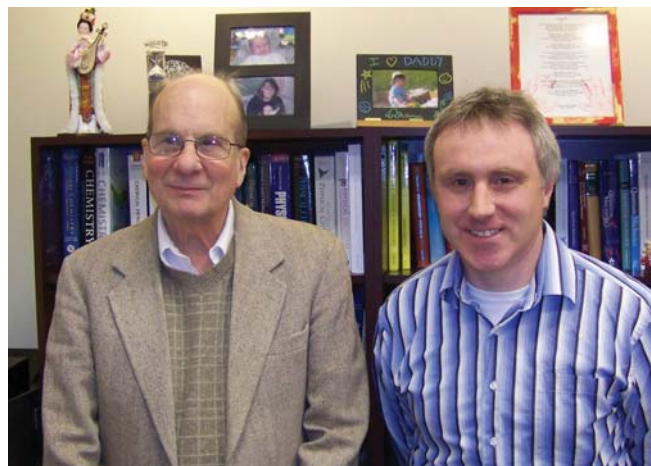
Our alumni are among the most supportive in the College and I want to thank all of our alumni for your continuing support of the Department for the past year. I have enjoyed meeting some of you the past three years and I sincerely hope to meet more of you during your visits to Rochester, or at one of the national ACS meetings next year. Our chemistry alumni around the country provide critical input into how to best advance Chemistry at Rochester and we appreciate the discussions. Finally, I wish to extend a personal invitation to return to Rochester for Meliora Weekend in 2016, with events running October 6th through the 9th. We will continue to have the annual Chemistry Department Gates Happy Hour on campus in the late afternoon on Saturday of Meliora Weekend. The Gates Happy Hour provides a special opportunity to acquaint yourself with current members of the Department and reconnect with old colleagues and classmates.

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

Sincerely,



Todd D. Krauss  
Professor of Chemistry and Chair  
Professor of Optics



*Todd and his Ph.D. research advisor, who was the W. Albert Noyes Memorial Lecturer, Cornell University Professor Louis Brus.*

# Donors 2014-2015

\* INCLUDES 2013-14 GIFTS TO THE  
DEAN'S FUND FOR CHEMISTRY

## GIFTS OF \$500,000+

Louis G. Lange III (B.A. '70)

## GIFTS OF \$100,000+

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Margaret H. Tsay

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Edward J. (Ph.D. '66) and Lenore Grabowski  
James L. Robo and Meredith B. Trim  
Margaret May-Som Wu (M.S. '74, Ph.D. '76) and  
Wuu-Yong Wu (Ph.D. '74)

## GIFTS OF \$5,000 - \$9,999

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Thomas O. Shannon (B.A. '84)\*

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Marcia and Professor Richard S. Eisenberg  
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Samir Farid  
Richard S. Foggio (B.S. '81)  
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Ph.D. '01)  
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*Clock Tower in Dandelion Square*





Kevin Guertin (Flw`93)  
Henry A. Havel (B.S.`76)\*  
Thomas A. Henderson (M.S.`83, Ph.D.`86)  
John K. Jenkins (Flw`71)  
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    Richard A. Josephson (B.A.`77)  
Joyce P. Kaisa (B.S.`92)\*  
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    Dieter A. Knecht (Ph.D.`68)  
Elliot Krauss (B.A.`74)  
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Norman A. Leister (Ph.D.`58)\*  
Frederick D. Lewis (Ph.D.`68)  
Lanny S. (M.S.`74, Ph.D.`77) and  
    Diane Liebeskind  
William J. Linn (Ph.D.`53)  
Dean C. Marvin (B.A.`73)  
Paul C. (M.S.`77, Ph.D.`79) and Stella K. Naegely  
Anita V. Pavels (B.S.`76, M.D.`80M)\*  
Thomas J. Perun (Ph.D.`63)  
Paul D. Sleezer (B.S.`58)  
Bruce G. Stokes (M.S.`75, Ph.D.`77)\*  
Bruce M. Szabo (M.S.`89) and Julie Rehm  
(M.S.`93, Ph.D.`96)\*  
Patricia (M.S.`84) and James Tata\*(M.S.`84,  
    Ph.D.`88)

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Marvin L. (B.S.`56) and Barbara S. Becker  
David A. Bittker (Ph.D.`53)\*  
Virginia B.(Ph.D.`64) and  
    Edward A. Caress (Ph.D.`63)  
Donald T. Culley (B.S.`58)\*  
Julie A. Eklund and Scott M. Kampmeier  
Deborah Graves (B.S.`82, M.S.`84, Ph.D.`88)  
    and Jeffrey Wood (M.S.`82, Ph.D.`86, Flw`88)  
Richard (B.S.`68, Flw`74) and  
    Annette Jaffe (Flw`74) \*  
Shyam Karki (M.S.`91, Ph.D.`95)  
Catherine L. Lawson (B.S.`82) and  
    Edward W. Castner Jr. (B.A.`82)  
Roy A. Leckonby (M.S.`74, Ph.D.`76)  
Ronald M. Levinson (B.S.`56)  
Margaret Logan (M.S.`72, Ph.D.`82, Flw`88)  
Doris W. (B.A.`50) and  
    George W. Luckey (Ph.D.`50)  
Elena Nilosek (M.S.`12, Ph.D.`15)  
James B. Philip, Jr. (M.S.`78, Ph.D.`81)  
Zachary K. and Shannon Sweeney  
Mildred Y. (Ph.D.`59) and Robert Tain  
Ronald R. Valente (M.S.`85, Ph.D.`88)\*  
Sanford T. (Ph.D.`63) and Margaret Young

# Donors 2014-2015

## OTHER GIFTS

Cameron Ainsworth (Ph.D. '49)\*  
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Kristen Bentley (B.S. '14)  
Wesley E. Bentz (Ph.D. '71)  
Peter R. Bernstein (B.S. '73) and Ala Hamilton-Day  
Sylvia L. Betcher (B.A. '70)  
Sarah Bugner (B.A. '14)\*  
Melissa P. Cardona (B.S. '13)\*  
Arthur E. Chin (B.S. '71, Ph.D. '78)\*  
Noal (B.S. '59) and Ann B. Cohen  
Christopher J. Collison (Flw '00)  
Mark S. (B.S. '79) and Deborah Connolly  
Kenneth R. Connor Jr. (B.S. '77) and  
Patricia E. Connor  
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Steven A. Dombchik (B.S. '64)\*  
Robert Eilerman (M.S. '71, Ph.D. '75)  
Richard P. English (B.S. '65)  
Kimberly Estep (M.S. '85, Ph.D. '88)  
Tinguan Gao (M.S. '04, Ph.D. '08)  
Hyman Gesser (Flw '53)\*  
Edward M. (M.S. '83, Ph.D. '87) and  
Janet Gordon (M.D. '85)\*  
Elliott S. (B.S. '72), (M.D. '77M) and  
Nancy M. Green  
Kenneth F. Greenough (Ph.D. '60)\*  
Alison K. Hamlin (B.S. '13)\*



Eve S. Hamlin\*  
David J. Hart  
William P. Hauser (Ph.D. '61)  
Eric Herbst (B.A. '66)  
Alison J. Hulchanski (B.S. '09)\*  
Nicholas Jacob (B.S. '13)  
Curtis E. Johnson (Flw '85)\*  
Joan E. (B.A. '64) and  
Alexander L. Johnson (Ph.D. '64)  
Nicole A. Ketterer (B.S. '03)\*  
Peter Krasniak (B.S. '14)\*  
Kathryn Leach (M.S. '05, Ph.D. '09)\*  
Kathryn M. (B.S. '09) and  
Brendon M. Lyons (B.S. '08, M.S. '09)  
Mark E. (M.S. '82, Ph.D. '85) and Mary McGuire  
Ronald H. Micheels (B.S. '72)  
Steven Moskowitz (B.S. '93)\*  
Deborah Z. (B.S. '85) and  
Thomas P. Nifong (M.D. '95M)  
Moriah (B.S. '08) and  
David Nissan (B.A. & B.S. '08)\*  
David Ochola (B.A. '88)\*  
Mikael Olezeski (B.S. '13)  
Cynthia Palmer (B.A. '74)\*  
Sofia Papatheodorou (B.S. '61)\*



## IN MEMORIAM

*The Department of Chemistry  
mourns the passing of:*

William George Drelles (B.S. '07)  
David H. Edison (Ph.D. '59)  
Frederick C. Loveless (Ph.D. '58)  
Elbert Dickerson Nostrand (Ph.D. '54)  
William R. Nummy (Ph.D. '50)  
Marguerite "Peg" Pomeroy (staff)  
John M. Ross (Flw '55)  
Edwin Albert Spath (B.A. '69)  
Charles J. Wright (Ph.D. '55)

Rachel Park (B.S. '14)\*  
Clyde Riley (B.S. '60)\*  
Brian Rohrs (B.S. '83)  
Andre Rosowsky (Ph.D. '61)\*  
Pamela L. Russ (B.S. '63)  
Abbas Shikari (B.S. '14)\*  
Albert H. Soloway (Ph.D. '51)  
Priscilla Stanley (B.A. '68)\*  
Samuel S. (Ph.D. '64) and Janice A. Stradling ('62N)  
Bruce M. Szabo (M.S. '89)  
Yuchen Tang (M.S. '04, Ph.D. '07)  
Johnson Truong (B.S. '15)  
Barbara Vasselli (B.A. '47)\*  
Paul Wermer (B.S. '76)\*  
C. Richard Zobel (Ph.D. '55)\*

## FOUNDATIONAL

Fidelity Charitable Gift Fund  
Leukemia & Lymphoma Society  
Schwab Charitable Fund  
MBL Family Foundation  
Canandaigua Kiwanis Foundation Inc.



**DONALD HULTQUIST (B.S. '56, Ph.D. '62)** received



a B.S. in Chemistry in 1956 and a Ph.D. in Biochemistry in 1962. Prof. Ralph Helmkamp supervised his project titled "Separation of Straight-Chain from Branched-Chain Molecules using Zeolites. For his Ph.D. thesis, he characterized lactoperoxidase and its unique heme prosthetic group.

As a post-doc at the University of Minnesota and then at UCLA, Don worked in the laboratory of Nobel Laureate Paul Boyer and identified, for the first time, phosphohistidine in mammalian tissues. He then served as a faculty member at the University of Michigan Medical School for 38 years. Don retired to Oberlin, Ohio and now serves as an Affiliate Scholar at Oberlin College, continuing, on a reduced scale, to lecture, interact with students, and collaborate on research.

Don hopes that Professors Helmkamp, Boekelheide, Gates, Wiig, Bond, and Saunders would be pleased that they taught him enough aromatic, heterocyclic, and transition metal chemistry to set him on the track of making research contributions to tetrapyrrole chemistry, redox enzymology, and prevention of tissue oxidative damage. He also hopes that they would be pleased to know that emulation of these teachers served him well in developing teaching techniques for the training of thousands of medical students and graduate students.

Don is likewise indebted to the U of R (Strong Memorial Hospital in particular) for giving him the opportunity to meet a young occupational therapist named Nancy who became his life-partner.

**MARK ROCHKIND (B.S. '62, Chemistry Faculty '65-66)** earned a Ph.D. in Chemistry at Berkeley and spent 17 years at Bell Laboratories followed by 10 years at Philips Electronics as President of Philips

USA Research Laboratories and then as an Executive at Philips Lighting in Eindhoven, Netherlands. Following 5 years at AT&T as an R&D Executive, he retired in 1998. The Rochkind-Wagner Foundation funds awards for very high performing math and science students at selected public high schools in NJ.



The picture shows Mark and his wife Pat in front of the mountaintop 169' buddha which overlooks Thimphu, capital of Bhutan.

**RICHARD "DICK" ENGLISH (B.S. '65)** retired from the



"real" world over a year ago. His wife, Anita, and their Golden Retriever, Reilly, are enjoying shuttling between their permanent home in Aptos, CA and their winter and summer retreat in Ketchum, ID. Dick and Anita skied 50 days last winter and are

looking forward to an even snowier and better skiing season this year. They love hiking, biking, and just being in the mountains of Southern Idaho. Dick is working towards returning to playing tennis after a very long hiatus, he loves reading, and is also studying the guitar after a teenage fling with the instrument. As the lack of water has become a major concern in California and elsewhere in the West, he has been trying to understand the challenges while keeping a few brain cells connected to something involving technology.

**PETER R. BERNSTEIN (B.S. '73)** is the founder and Principal at PharmaB LLC, a consulting firm dedicated to the discovery and development of new, safe and effective pharmaceuticals. Peter also holds multiple editorial and academic appointments. Most notably, he is the BMCL Digests Editor for



Bioorganic & Medicinal Chemistry Letters, Section Editor for Annual Reports in Medicinal Chemistry, and is an Adjunct Professor of Chemistry & Biochemistry at the University of Delaware. He was chosen as the "Distinguished Lecturer" for the 2010 AstraZeneca Excellence in Chemistry Award and in 2011 he was named to the ACS Division of Medicinal Chemistry Hall of Fame. In 2016, he will be the Chairman of the Tetrahedron Symposium in Sitges, Spain.

Peter R. Bernstein earned his Ph.D. with Professor Gilbert Stork at Columbia University in 1977. He then served as an Organic Chemistry Fellow in the laboratory of Professor Barry Trost in the Department of Chemistry at the University of Wisconsin, Madison. In 1979, Peter joined the Medicinal Chemistry Department of ICI Pharmaceuticals Group in Wilmington, DE. He worked there 31 years, continuing through its spin-off as Zeneca Pharmaceuticals and through its merger with Astra Pharmaceuticals to form AstraZeneca Pharmaceuticals.

**JOHN C. MOORE (B.S. '74)** graduated in 1974 with a B.S. in General Science with an emphasis in Chemistry. John is most grateful for one chemistry course; Physical Organic Chemistry. The University taught him how to solve problems. Currently John is the CTO of TearSolutions, a development-stage biotechnology company that is advancing a novel, first-in-class topical treatment for dry eye. The drug is a synthetic fragment of the human tear protein, lacritin, that promotes tearing and reduces cellular stress to restore corneal health and reduce inflammation. He also serves as Chairman of the Board of Optovue, a global leader in the development and commercialization of optical coherence tomography (OCT) and OCT angiography technology for the eye care market. In addition, John is a member of the Board of STAAR Surgical, the leading provider of phakic IOLs (implantable lenses).

**BARBARA J. BURGER (B.S. '83)** is president of Chevron Technology Ventures (CTV), a role she has held since June 1, 2013. CTV sponsors the scouting, demonstration and integration of emerging technologies into Chevron.

Joining Chevron in 1987, Burger started as a research chemist at the Richmond Laboratory. After several technical assignments, she went on to a number of management positions of increasing responsibility in International Marketing, Chemicals, Technology Marketing and Lubricants.

Burger currently serves on the board of directors for the Houston Technology Center, a technology and business incubator, and is a governing board director, member of the Executive Committee and chair of the Finance Committee of the Houston Symphony Society. She also serves on the U.S. Department of Energy National Renewable Laboratory External Advisory Council as well as on the governing board for the MIT Energy Initiative. Burger served as a non-executive director for Caltex Australia Limited, an ASX100 company, from 2012 to 2015.

An active alumna of the University of Rochester, Burger joined the Board of Trustees in 2015. She is a member of the university's San Francisco Bay and Texas Regional Cabinets, the university's River Campus Libraries National Council and is a member of the George Eastman Circle, the university's leadership annual giving society. In 2012, she established the Barbara J. Burger Endowed Scholarship in the Sciences to support students pursuing degrees in biology, chemistry, earth and environmental sciences, or physics.

Burger graduated with a bachelor's degree in chemistry from the University of Rochester in 1983. She went on to receive a doctoral degree in chemistry from the California Institute of Technology in 1987 and an academic honor M.B.A. in finance from the University of California, Berkeley in 1994.





**DR. JOSEPH SWIDER (B.S. '91)** earned a B.S. in Chemistry and Art History from the University of Rochester in 1991 and a Ph.D. in Nuclear Chemistry from the University of Maryland at College Park in 1998. His doctorate research utilized a novel cold-

neutron analytical technique for chemical analysis of small samples and artists' materials. During a portion of his graduate studies he was employed by the Science Department at the National Gallery of Art in Washington, DC. There he provided analytical support for the Conservation Department and maintained the department's resin aging research. In 1998 he received a National Research Council Postdoctoral Fellowship at the National Institute of Standards and Technology in Gaithersburg, MD where he developed a new micro X-ray fluorescence instrument. Following his fellowship, he was employed as an Andrew W. Mellon Research Scientist of East Asian Paintings Research at the Freer Gallery of Art and Arthur M. Sackler Gallery of the Smithsonian Institution. Since 2004, Dr. Swider has been a senior research scientist at McCrone Associates in the Electron Optics Group in Chicago. He routinely uses scanning electron microscopy equipped with energy dispersive X-ray spectrometry (SEM/EDS) to analyze samples from art and archaeology, pharmaceutical, food, cosmetic, manufacturing, paint, polymer and forensic clients.

**ALISA THAVIKULWAT (B.S. '09)**

graduated from the University of Rochester School of Medicine in May 2015 and is currently completing her intern year at Medstar Harbor Hospital in Baltimore, MD. Alisa is interested in ophthalmology research with a focus on macular degeneration and vision disorders. Alisa is also part of the Medical Research Scholars Program at the NIH and was chosen to participate in the LabTV program which seeks to profile young scientists to serve as an inspiration for the younger generation. Short video profiles of Alisa and other young researchers are available at the website [www.labtv.com](http://www.labtv.com). In July 2016 she will begin her residency training in ophthalmology at the Eye and Ear Infirmary of the University of Illinois at Chicago.



**EMILY HART (B.S. '12)** is currently teaching General and AP Chemistry at KIPP NYC College Prep in the South Bronx. She loves teaching and is very excited to teach the AP curriculum this year. Emily is so thankful for everything she learned at Rochester that prepared her to be the teacher she is today. Emily was the 2012 recipient of the Presidential Award for Community Service which was established by the Dean of Students in 1990 to recognize University students who are committed to community service. Emily was obviously a perfect choice for that award!



KIPP NYC is a network of free, open-enrollment public charter schools preparing students for success in college and in life. KIPP (Knowledge is Power Program) schools incorporate what the KIPP founders learned from America's best, most charismatic teachers: lessons need to be lively; school days need to be longer (the KIPP day is nine and a half hours); the completion of homework has to be sacrosanct (KIPP teachers are available by telephone day and night). KIPPsters in New York are dramatically outpacing their peers with respect to high school graduation and college matriculation and graduating college at 4 times the rate of low-income students nationally.

**RICHARD E. PARTCH (Ph.D. '62)**

a senior university professor with Clarkson University's Center for Advanced Materials Processing (CAMP), has been named a fellow of the American Chemical Society. ACS Fellows are nominated by their peers and selected for their outstanding achievements in and contributions to science, the profession, and the Society.



Professor Partch, a native of California, attended Pomona College in that state for his B.A. degree majoring in chemistry. He then studied for his Ph.D. (1962) with research advisor Professor Marshall Gates in the area of medicinal organic chemistry at the University of Rochester. From 1962-65 he served as Assistant Professor at New Mexico Highlands University then moved to Clarkson University in Potsdam, NY where he has served from 1965 as Associate, Full and now Senior University Professor, and from 1968-73 as Chemistry Department Executive Officer. Since 1990 he has been a recognized contributor to the success of Clarkson's Center for Advanced Materials Processing. Partch has received research funding of more than \$5 million from industry, as well as many branches of government.

Partch, who completed his 50th year at Clarkson in June, was recognized for mentoring youth to understand the importance of fundamental academic and applied government and industrial advances that only chemists can achieve. He was also cited for his more than 40 years of volunteer outreach to high school science teachers and their students throughout the United States and sharing how chemistry impacts every aspect of life.



**FREDERICK LEWIS (Ph.D. '68)**, a professor emeritus of chemistry at Northwestern University in the Weinberg College of Arts and Sciences, was honored with the 2016 Josef Michl ACS Award in Photochemistry. Lewis' research involves understanding the relationship between the unique structure of DNA and its interaction with light.

Professor Lewis received a B.A.

in Chemistry from Amherst College in 1965, a Ph.D. from the University of Rochester in 1968 with advisor William Saunders, and moved on to the laboratory of Nicholas J. Turro at Columbia University as a NIH postdoctoral fellow. He has been at Northwestern University since 1969, rising quickly through the ranks to become a full professor and a very active member of the photochemical community. He has served on several professional advisory and review boards and symposia organizing committees, as well as being an editor for several journals. A reunion for former members of his research group and colleagues was held in July 2013 to

celebrate his retirement and 44 years of photochemical research.

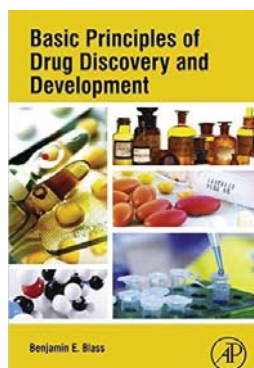
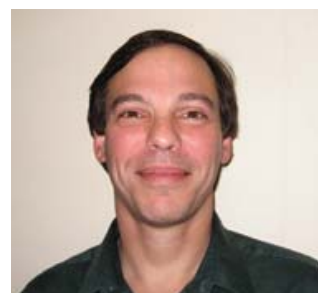
After thoroughly enjoying his four years at the University of Rochester learning more chemistry than he thought was possible under Chris Dalton, Andy Kende, Jack Kampmeier, Bill Saunders, Louie Friedrich, and Dick Schlessinger, **ROBERT BOURQUE (Ph.D. '80)** took a career turn after getting his Ph.D. in Organic Chemistry in 1980, and went to law school — but did not leave his chemistry training, or his love of chemistry behind. Bob spent his career at a New York City law firm, Simpson Thacher & Bartlett, where he co-founded both the Environmental Practice and the Intellectual Property Practice. He spent the bulk of his time representing pharmaceutical and other biomedical companies in litigation and counseling — often needing to draw on his organic chemistry background. Bob retired from practicing law in 2010, but does a bit of consulting for early-stage biomedical companies, and volunteers his time with several environmental organizations.

**BENJAMIN BLASS (Ph.D. '94)** received his B.S. in

Chemistry from Emory University in 1990 and his Ph.D. in Organic Chemistry in 1994 from the University of Rochester under the direction of Andrew S.

Kende. Upon completion of his doctoral program, Dr. Blass pursued a career in drug discovery and development with Procter & Gamble Pharmaceuticals (1994-2006) and Wyeth Research (2006-2010). Over the course of his industrial career, Dr. Blass conducted research on a wide range of disease states through the careful application of medicinal chemistry strategy and drug design principles. He is the principal author or co-author on seventy patents, publications, and invited lectureships and is registered with the United States

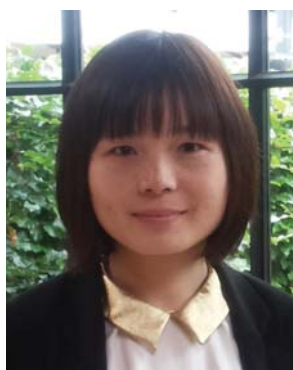
Patent and Trademark Office as a patent agent. He is currently an Assistant Professor of Medicinal Chemistry at the Moulder Center for Drug Discovery Research at the Temple University School of Pharmacy. He has just published his first textbook titled “Basic principles of drug discovery and development.”





President Barack Obama nominated **DR. KRISTEN KULINOWSKI (M.S. '92, Ph.D. '95)** as a member of the Chemical Safety and Hazard Investigation Board (CSB) in January 2015, and she was confirmed by the Senate in August 2015. Dr. Kulinowski is an adjunct assistant

professor in the Department of Chemistry at Rice University. She currently works in Washington DC at the IDA Science and Technology Policy Institute (STPI), a federally funded research and development center that provides analytical support to the White House Office of Science and Technology Policy and other Federal agencies. Prior to joining STPI in 2011, she was at Rice University as Senior Faculty Fellow in Chemistry, Executive Director for the Center for Biological and Environmental Nanotechnology (CBEN) and the Director of the International Council on Nanotechnology (ICON). Dr. Kulinowski published the first database of citations to peer-reviewed papers addressing nanomaterial risks, a survey of best practices for nanomaterial workplaces, and the GoodNanoGuide, an interactive forum for sharing information about nanomaterial handling practices. Dr. Kulinowski received a B.S. degree in chemistry with honors from Canisius College and M.S. and Ph.D. degrees in chemistry from the University of Rochester in the research group of Professor Anne Myers Kelley.



Congratulations to 2014 Ph.D. graduate **DR. YUNZHE JIAO (Ph.D. '14)** for being selected as one of the 45 finalists for the Elsevier Reaxys Ph.D. Prize. Selected from over 450 submissions from around the globe, these 45 talented chemists join the Reaxys Prize Club; a community of

inspiring minds making meaningful contributions to chemistry. All 45 finalists were invited to present their research at the 2015 Reaxys Ph.D. Prize Symposium, September 7-8, 2015, in Hong Kong. In its sixth year, the Reaxys Ph.D. Prize recognizes chemistry Ph.D. students and recent graduates, the prize continues to foster creativity in groundbreaking chemistry by identifying the chemistry leaders of tomorrow.

Yunzhe Jiao graduated from Nankai University with a B.S. degree in Chemistry in 2009. She came to the University of Rochester in August 2009 and began her graduate studies in organometallic chemistry under the supervision of Prof. William D. Jones. Her Ph.D. thesis covered organometallic, inorganic, and organic chemistry, and was accepted in June 2014. It focused on reactivity evaluation of transition metal systems towards homogeneous C-H activation as well as selectivity control and mechanistic study with experimental and computational methods. She joined SynCat@Beijing in January 2015.



**SALVATORE F. PRIORE (M.D., Ph.D. '15)** is currently a Resident Physician at the Hospital of the University of Pennsylvania Department of Pathology & Laboratory Medicine. Sal received an M.D. from the University of Rochester School of Medicine

and Dentistry in May 2015 and also his doctoral degree in Chemistry after working in Doug Turner's research group. His research interests include the global analysis of RNA structure in disease states using next-generation sequencing methods and the application of bioinformatics methods to study RNA evolution, codon usage, and structure from next-generation sequencing data.

**GONZALO GUIRADO (Flw '03-04)**, who was a postdoctoral fellow and is a current collaborator with Professor Dinnocenzo's Group, has been Coordinator of the Ph.D. Program in Chemistry at the Autonomous University of Barcelona (UAB) in Barcelona (Spain) from 2011 to 2015. He was awarded with the first APOSTA UAB prize in the environmental category for his research into "Electrochemical Sustainable Strategies for Reducing the Impact of Carbon Dioxide using Ionic Liquids". Gonzalo and Elisabeth welcomed their first daughter, Mireia, in May.





# Focus on Class of 1975

## STEVEN J. SIBENER (B.S.

'75), the Carl William Eisendrath Distinguished Service Professor at The University of Chicago, received his B.S. in chemistry and B.A. in physics in 1975 from the University of Rochester, and his M.S. (1977) and



Ph.D. (1979) degrees in chemistry from the University of California, Berkeley, under the guidance of Nobel Laureate Yuan T. Lee, the master of molecular beam chemistry. After accepting appointment as Assistant Professor of Chemistry at The University of Chicago while still a graduate student, he then continued his research as a postdoctoral fellow at Bell Laboratories. He started his independent academic career in 1980 at Chicago, and has remained there ever since.

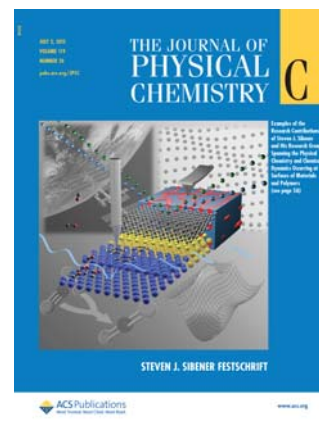
While at Rochester he conducted theoretical studies on the shape of liquid interfaces, conducting his undergraduate thesis research under the guidance of Professor Frank Buff. The class of 1975 was the last to take freshman chemistry in Lattimore Hall, and the first to take classes in Hutchinson Hall.

He has served as Director of The James Franck Institute, the NSF Materials Research Science and Engineering Center, the DoD Center for Materials Chemistry in the Space Environment, and the multi-university NSF Center for Energetic Non-Equilibrium Chemistry at Interfaces. He has chaired the two faculty committees that recommended forming the new Institute for Molecular Engineering and defined its ambitious horizons. He is currently a Fellow of the Institute for Molecular Engineering (IME), as well as Director of the University of Chicago's IME Water Research Initiative.

Professor Sibener was surprised by many of his students, postdocs and colleagues who arranged a two-day "SibenerFest" in honor of his 60<sup>th</sup> birthday in March 2014. A special Festschrift Issue of the Journal of Physical Chemistry C (July 2nd, 2015) celebrating Steve's numerous innovative and influential scientific achievements contains an exciting collection of articles from researchers around the world as a tribute to his enduring science, creativity, leadership and friendship.

Steve has made seminal contributions to a wide variety of forefront areas of modern chemistry encompassing chemical physics, surface and materials chemistry, catalytic reaction kinetics, polymeric systems, and nanoscience. His contributions have focused on elucidating the atomic-level dynamical properties of interfaces, as well as the chemical processes and transformations that occur on such interfaces. Molecular beam scattering, scanning probe microscopy imaging, numerical simulations and theory all play prominent roles in his research. He is especially proud of the accomplishments achieved by the many outstanding postdoctoral fellows, graduate, undergraduate, and high school students who have participated in his research program. He has served as doctoral advisor for Rochester chemistry undergraduates Kevin Peterlinz and, currently, Jonathan Raybin, as well as publishing with recent Rochester undergraduate Sara Rupich.

Amongst his many honors are the Marlow Medal of the Royal Society of Chemistry and the Arthur W. Adamson Award for Distinguished Service in the Advancement of Surface Chemistry of the American Chemical Society. He is a Fellow of the American Physical Society and the American Association for the Advancement of Science, and has been twice elected a Visiting Fellow of the Joint Institute for Laboratory Astrophysics.



# Focus on Class of 1975

Louisiana State University Chemistry Professor **GEORGE STANLEY (B.S. '75)** always seems to have a smile on his face, especially when he is putting on a demonstration for middle and high school students. He has made science and chemistry education and outreach his priority as demonstrated by his coordination of Super Science Saturday (SSS), an annual event that celebrates National Chemistry Week that was first held in 1987 at a mall, moved to LSU 15 years ago and recently hosted up to 1000 K-12 students and 1500 parents this past fall. There were 19 stations with hands-on demonstrations and activities to engage students and adults alike. Each K-12 student that attends is given a Passport at the check-in area that has blocks for all the activity stations. When the student visits the station and participates in the activities the Passport is stamped. After visiting all the activity stations they receive some small gifts at the check-out area. The event is sponsored by the Baton Rouge section of the ACS, the LSU Department of Chemistry, and LSU Athletics. Several local chemical companies had employees conducting experiments.

Professor Stanley is also very involved in a new education effort between LSU Chemistry and Dow Chemical that has two major plants within an hour's drive from the university (Dow Plaquemine and their St. Charles plant at Taft, LA). Below are a couple of photos of him teaching chemistry for the Dow Chemical "Bring your Child to Work" event at their Taft chemical plant on July 29, 2015. He took 10 LSU chemistry graduate students and two undergrads to staff 6 activity stations for 2 hours of hands-on chemistry demonstrations for the 56 middle and high school aged children that attended the event.



The demonstration activities that they did are part of the ChemDemo (chemistry demonstration) service-learning program that sends 600 to 800 LSU students a semester (mostly undergrads taking our general chemistry classes) out to teach 50 minute classes in regional K-12 schools. Professor Stanley started the ChemDemo program in 1997 and since then they have sent out 13,782 LSU students who visited 6,575 regional classrooms impacting over 162,000 K-12 students. This is one of the largest chemistry outreach and education programs in the US.



*LSU Dean of Science Cynthia Peterson with George Stanley on Super Science Saturday 2015.*

Professor Stanley received his Ph.D. in Chemistry from Texas A&M in 1979 and traveled to Strasbourg, France as a NATO and CNRS postdoctoral fellow for two years. After five years at Washington University in St. Louis, he moved on to LSU in 1986, and moved quickly up the ranks to his current position of Cyril and Tutta Vetter Alumni Professor. His research interests include inorganic and organometallic chemistry directed towards new industrially relevant catalysts which began during his undergraduate research in the Eisenberg group.



## Department Mourns the Loss of Esther Conwell

The department continues to mourn the loss of Professor Esther Marly Conwell, known for her groundbreaking work on semiconductors and her mentorship of women in science, who was born in New York City on 23 May 1922 and died in Rochester, New York, on 16 November 2014. Professor Conwell was married to the novelist Abraham Rothberg, who died in 2011. She is survived by her son, fellow scientist Dr. Lewis J. Rothberg, professor of chemistry, physics and chemical engineering at the University of Rochester, his wife, Shelby Nelson, and their two children, Charles and Vivian.

Over the course of her 70-year research and teaching career, she made foundational contributions to many emerging areas of science, including the electrical properties of semiconductors, light propagation in optical fibers, and charge motion in quasi-one-dimensional materials. She gravitated toward controversial and novel scientific areas and thrived on scientific debate. Her efforts were marked by a tenacity and focus that kept her involved in research throughout her life; at the time of her death, she still had papers out for journal review and was drafting an article on charge transport in DNA.



*Esther Conwell*

Esther received her B.S. degree in physics from Brooklyn College in New York City in 1942. She was blessed with mentors who recognized her talent and encouraged her to continue with graduate education. Her master's thesis, on the theory of impurity scattering in semiconductors, was done with Victor Weisskopf at the University of Rochester. Remarkably, Esther completed this signature work in a few months, as Weisskopf was being sent to Los Alamos to aid in the war effort there. That highly influential work, now known as the Conwell–Weisskopf formula, helped underpin the development of the transistor and other semiconductor devices. Her Ph.D., completed in 1948 with Subrahmanyan Chandrasekhar at the University of Chicago, was on quantum computations of astrophysically important negative ions such as those of hydrogen and oxygen.

After teaching physics at Brooklyn College until 1950, Esther worked as a postdoctoral fellow with William Shockley at Bell Labs and helped to develop the theory of “hot electron” transport in germanium. She continued her research on charge transport at Sylvania Research Laboratories and General Telephone Laboratories from the late 1950s through the late 1960s. Her monograph on high-field transport was influential in the development



*Esther with Lewis, Shelby, Charles, and Vivian.*

of semiconductor electronics. She also made important early contributions on wave propagation in optical fibers. During that period she began encouraging young women to become scientists.

Esther moved to Xerox in Webster, New York, in 1972. She initially joined and ultimately led a program on integrated optics. When that program was relocated to Xerox PARC in California, she remained at Webster, where she joined a group for theoretical physics and chemistry and began studying the transport and optical properties of quasi-1D organic semiconductors such as TTF-TCNQ. Esther played a crucial role in the emerging field of organic electronic materials and published seminal papers on the theory of the mobility and optical properties of polaronic charge carriers in conjugated polymers and organic semiconductors. Her research was an important part of a substantial effort at Xerox to develop flexible-belt photoreceptors, which became the basis for a highly successful series of products in the 1980s and 1990s. She was known to her colleagues for her unwavering devotion to her ballet lessons every Friday morning and her preparation of popcorn all day, every day, at the office.

In 1989 Esther helped bring to the University of Rochester the NSF Center for Photoinduced Charge Transfer, a collaborative effort of Xerox, Eastman Kodak, and the university. She later served as the center's associate director and became an adjunct faculty member in the university's department of chemistry. After retiring from Xerox in 1998, Esther continued working at the university, where she brought theoretical insight to the diverse experimental results on charge transport in DNA, another quasi-1D semiconductor. She promoted the controversial concept of polaronic



*Esther Conwell*

charge conduction along DNA molecules and supported her ideas with quantum chemical calculations.

Esther's innovative semiconductor research earned her a place as one of Discover magazine's 50 Most Important Women of Science in 2002. As a successful and highly influential woman in the physical sciences, she inspired and mentored countless young women to pursue and grow in scientific careers. The American Chemical Society acknowledged those aspects of her influence in 2008 with its Award for Encouraging Women into Careers in the Chemical Sciences. Even half a century later, Esther's scientific breakthrough work on



*Esther with President Joel Seligman and Professor Boeckman.*



*Esther receiving the National Medal of Science from President Obama in 2010.*

semiconductors is still important to the understanding of electron transport today. Esther helped launch the computer revolution by explaining the effect of impurities and of high electric fields on electron travel through semiconductors. Her research earned her membership in the National Academy of Sciences, the American Academy of Arts and Sciences, and the National Academy of Engineering, among the highest honors a scientist or engineer can receive. Esther is the only member of the University of Rochester to hold such a distinction.

Esther's exceptional scientific contributions were recognized with the IEEE Edison Medal in 1997 and the National Medal of Science given to her by President Obama in 2010. The President commemorated Esther for "her broad contributions to understanding electron and hole transport in semiconducting materials, which helped to enable commercial applications of semiconductor and organic electronic devices, and for extending her analysis to studying the electronic properties of DNA." Robert K. Boeckman, Jr, former chair of the Chemistry Department, said that "when Esther learned of the award, she was concerned that the activities might delay submission of her next journal article. When the UR press group sought to meet with her, she scheduled them around her student meetings. For the actual UR press announcement, she was glad it came after a student's poster session she was attending. For Esther, it was always about the science."

Although Esther no longer taught chemistry courses at the university, she still worked almost daily on campus and was considered a mentor by both undergraduate and graduate students and fellow faculty members, said Todd Krauss, current chair of the chemistry department. A memorial service to celebrate her life was held on March 6, 2015 at the Interfaith Chapel on the University of Rochester campus, and it was attended by many of Esther's colleagues, former and current students, friends and family. As Todd mentioned in his remembrance of Esther, he will miss seeing her gold Buick Century parked in the same parking spot in Trustee Lot, knowing that she was hard at work in her 4th floor office in pursuit of the answer to the question of how charges move in DNA. We will all miss her high standards, uncompromising honesty, forthright approach to science, and love of students.

Earlier this year, the Esther M. Conwell Graduate Fellowship Fund was established by her son and faculty member, Lewis Rothberg (B.S.'77) and his wife Shelby Nelson. The fund was created in memory of Esther's accomplishments to the Department of Chemistry and will provide stipend support for merit-based fellowships for advanced (third year or beyond) graduate students pursuing a Ph.D in Chemistry who show exceptional promise as researchers. Dr. Rothberg and Ms. Nelson have also created a matching gift component to this fund, where they will match up to \$20,000 in a calendar year any gift that is designated to the Conwell Graduate Fellowship Fund. If you would like to contribute, the money you give will multiply when it is matched by this challenge grant.



## David MacMillan Receives 2014 Harrison Howe Award



*David MacMillan receiving the Harrison Howe Award from ACS Rochester Section President Glen Labenski, and Brad Nilsson*

**The 2014 Harrison Howe Award of the Rochester Section of the American Chemical Society was presented to Professor David W. C. MacMillan** on May 7<sup>th</sup>, 2015 at the University of Rochester. The event is a semiannual highlight of the local chemistry community that commemorates ACS Rochester Section cofounder Harrison E. Howe by recognizing a prominent scientist who has made outstanding contributions in chemistry, as well as demonstrated potential for further achievement. Professor Bradley Nilsson is the current chair of the Harrison Howe Award Committee, which also includes Professor David McCamant as a member.

Professor MacMillan is recognized as the leader of the burgeoning field of organocatalysis. The MacMillan group has pioneered the use of chiral organic molecules as catalysts for stereocontrolled reactions. In a classic paper, MacMillan reported in 2000 (*J. Am. Chem. Soc.* **2000**, *122*, 4243-4244) that chiral amines effectively catalyzed the formation of Diels-Alder products in high

enantioselectivity via chiral iminium activation. Since then, the MacMillan group has reported a stunning array of transformations based on the principle of iminium activation. This work has sparked a modern renaissance in the development of non-metal organocatalysts. MacMillan's work includes seminal achievements in iminium catalysis, enamine catalysis, cascade catalysis, asymmetric hydrogenation, and photoredox catalysis.

MacMillan received his B.S. in Chemistry in 1991 from the University of Glasgow and his Ph.D. in Chemistry in 1996 from the University of California, Irvine (Professor Larry E. Overman). He conducted postdoctoral studies with Professor David A. Evans at Harvard University from 1996–1998 prior to accepting an appointment at the University of California, Berkeley in 1998. He joined the Department of Chemistry at the California Institute of Technology in 2000 and subsequently moved to Princeton University in 2006. He is currently the Chairperson of the Department of Chemistry at

Princeton University and is the James S. McDonnell Distinguished University Professor of Chemistry. He has also been the Director of the Merck Center for Catalysis at Princeton University since 2006.

The Chemistry Department was pleased to host Professor MacMillan throughout his visit to Rochester, which included meetings with faculty in Chemistry and Chemical Engineering and members of the awards committee of the Rochester section of the ACS. He also met with local graduate and undergraduate students from the Rochester area. His lecture, held at the University of Rochester Medical Center in the Class of 1962 Auditorium, was entitled "The Application of Photoredox Catalysis to New Transformations in Chemical Synthesis." The evening award presentation and seminar were immediately followed by a student poster session and dessert reception in the Flaum Atrium.

The Harrison Howe Award is dedicated to the memory of Harrison E. Howe, 1881-1942, a cofounder of the ACS Rochester Section and a well-known chemist, editor,



*Kyle Rugg showing his poster to Professor Dan Weix*

and author. The award was established to recognize a scientist who has made outstanding contributions to chemistry or closely related fields and who shows great potential for further achievement. There have been 68 Harrison Howe Award winners, twenty-six of whom subsequently won a Nobel Prize (39%).



# Chemistry-Biology-Biophysics Cluster Retreat 2015



## The annual Chemistry-Biology-Biophysics Interface Retreat was held on May 28-29, 2015.

The Chemistry-Biology-Biophysics Interface Training Cluster works to increase interactions between groups doing work at the chemistry-biology interface in Arts, Sciences, and Engineering, and in the School of Medicine and Dentistry at the University of Rochester. The Cluster currently has research groups from the Departments of Chemistry, Biology, Biochemistry & Biophysics, Microbiology, Pharmacology, Biomedical Engineering, and Immunology. The primary medium for achieving the Cluster's goals is an annual Retreat that is funded by the University Committee for Interdisciplinary Studies (UCIS), also with support from the Department of Chemistry.

The featured speaker at this year's retreat was Cynthia Burrows, Distinguished Professor and Thatcher Presidential Endowed Chair of Biological Chemistry at the University of Utah. The Retreat started on the afternoon of May 28 with a talk by Prof. Burrows to an audience of about 50 students, postdocs, and faculty in Goergen Hall. The talk was titled: "Spirocycles and G-Quadruplexes: How the Chemistry of Guanine Oxidation Changes the Biology of DNA." The seminar presented Prof. Burrows' recent findings on the relationship between chemical modifications of nucleic acids and their three-dimensional structures, with implications for cancer biology. Her talk provided a fantastic example of interdisciplinary research combining chemistry and biology.

The Retreat reconvened at the Staybridge Suites Hotel the next day with a record 98 attendees. The day started with continental breakfast followed by a presentation

titled "LOCI® Technology - Advanced Immunoassays in a FLASH" by Dr. Jason Kellogg (UR Ph.D., '05) from Siemens Healthcare Diagnostics. This was followed by a panel discussion on career directions that included Cynthia Burrows, Jason Kellogg, Prof. Christina Goudreau Collison (UR Ph.D., '04, Professor at RIT's College of Science), and Weimin Kaufman from UR Ventures.

After a buffet lunch, graduate students from the Departments of Chemistry, Dermatology, and Biomedical Engineering gave talks on their research. Fourteen students and postdocs, including a visiting postdoc from SUNY Albany, presented posters on their research in a lively poster session. Much information was exchanged throughout the two days and new connections were made that can enhance research and training at the Chemistry-Biology-Biophysics Interface at UR. The Retreat gave all participants a broad overview of research related to biological chemistry and an appreciation of interdisciplinary approaches.



Keynote speaker Cynthia Burrows and Kara Bren



## 2015 Summer Research Fellowships for International Students



*Students and mentors (left to right) : Ulises Torres, Rudi Fasan, Leopoldo Mejía, Ignacio Franco, Viktoria Steck, Mike Neidig, Dieuwertje Modder, Kara Bren, Manjista Mukharjee, and Ted Pagano ( Assistant Director of the UR Center for Education Abroad)*

Professor Ignacio Franco initiated a Summer Research Fellowship program designed to provide outstanding undergraduates in Chemistry from all over the world the opportunity to conduct first class summer research at the University of Rochester. In this first version, we had applicants from Asia, Africa, Europe, North America and South America and accepted five top students:

Leopoldo Mejía (U. Antioquia, Colombia, Physical Chemistry)- Franco group

Dieuwertje Modder (U. Netherlands, Inorganic Chemistry)- Neidig group

Manjista Mukharjee (Calcutta U., India, Inorganic Chemistry)- Bren group

Viktoria Steck (Humboldt U. of Berlin, Germany, Organic Chemistry)- Fasan Group

Ulises Torres (UNAM, Mexico, Physical Chemistry)- Franco group

These students worked closely with a Faculty member in the Department for approximately 8-10 weeks. Through the program, they received a stipend to cover their living expenses and travel costs. The experience for both the students and their hosts has been terrific, and we look forward to watching these students become future scientific leaders.



*The Franco Group on a tour of the Laboratory for Laser Energetics.*

# Chemistry Welcomes Ellen Matson

Assistant Professor of Chemistry

Ph.D. 2013, Purdue University



## RESEARCH INTERESTS

Probing cooperative reactivity between non-traditional ligand platforms and earth-abundant transition metals, specifically the ability of these novel complexes to facilitate a wide range of organic transformations with industrial, environmental, and biological relevance. Synthesis of novel inorganic and organometallic complexes and investigation of their role in small molecule activation and catalysis.

## CONTACT

matson@chem.rochester.edu

**ELLEN MATSON** joined the Chemistry faculty in July 2015. Ellen earned her B.A. in Chemistry and B.S. in Science Education in 2009 at Boston University. She then moved to the Midwest to pursue her Ph.D. in Chemistry at Purdue University under the guidance of Suzanne C. Bart. During her time as a graduate student, Ellen helped expand the understanding of the synthesis and reactivity of low-valent uranium alkyl complexes. Her work culminated in a number of national recognitions, including the Iota Sigma Pi Anna Louise Hoffman Award for Outstanding Achievement in Graduate Research (2013) and the American Chemical Society Division of Inorganic Chemistry's Young Investigator Award (2014). After obtaining her Ph.D., Ellen accepted a Postdoctoral appointment at the University of Illinois at Urbana-Champaign in the new research group of Alison R. Fout. During her time as a postdoctoral scholar, Ellen developed a new ligand platform featuring a redox-flexible secondary coordination sphere to investigate the role of electronic tautomerization and proton-coupled electron transfer in small molecule activation of biomimetic, non-heme iron complexes.

Ellen is thrilled to start this new chapter in her career in the supportive and collegial Chemistry Department at the University of Rochester and is looking forward to developing a competitive research program with the hard work of highly motivated graduate students. Ellen will be teaching a number of inorganic chemistry courses for graduate students in the fall semester, including Group Theory (CHM 415) and Organometallics I (CHM 421).

## Selected Publications:

Nickel(II) Pincer Carbene Complexes: Oxidative Addition of an Aryl C-H Bond to Form a Ni(II) Hydride. E. M. Matson; G. E. Martinez; A. D. Ibrahim; B. J. Jackson; J. A. Bertke; A. R. Fout, *Organometallics*, **2015**, *34*, 399.

Facile Nitrite Reduction in a Non-Heme Iron System: Formation of an Iron(III)-Oxo. E. M. Matson; Y. J. Park; A. R. Fout, *J. Am. Chem. Soc.*, **2014**, *136*, 17401.

Reductive Elimination from Tetrabenzyluranium Mediated by an Iminoquinone Ligand. E. M. Matson; S. Franke; N. A. Anderson; T. D. Cook; P. E. Fanwick; S. C. Bart, *Organometallics*, **2014**, *33*, 1964-1971.

Oxidative Addition of Halogens to U(IV) Bis(Amidophenolate) Complexes. E. M. Matson; S. R. Opperwall; P. E. Fanwick; S. C. Bart, *Inorg. Chem.*, **2013**, *52*, 7295-7304.

Isolation of Iron(II) Aqua and Hydroxyl Complexes Featuring a Tripodal H-bond Donor and Acceptor Ligand. E. M. Matson; J. A. Bertke; A. R. Fout, *Inorg. Chem.*, **2014**, *53*, 4450.

Synthesis and Reactivity of Trivalent Tp\*U(CH<sub>2</sub>Ph)<sub>2</sub>(THF): Insertion vs. Oxidation at Low-Valent Uranium. E. M. Matson; W. P. Forrest; P. E. Fanwick; S. C. Bart, *Organometallics*, **2013**, *32*, 1484-1492.

Functionalization of Carbon Dioxide and Carbon Disulfide Using a Uranium(III) Alkyl Complex. E. M. Matson; W. P. Forrest; P. E. Fanwick; S. C. Bart, *J. Am. Chem. Soc.*, **2011**, *133*, 4948-4954.

# Chemistry Welcomes Pengfei Huo

Assistant Professor of Chemistry

Ph.D. 2011, Boston University



## RESEARCH INTERESTS

Physical and theoretical chemistry, Ab-initio dynamics for understanding chemistry and photo physics of solar energy conversion.

## CONTACT

huo@chem.rochester.edu

**PENGFEI (FRANK) HUO** joined the Chemistry faculty in July 2015. Frank received his B.S. in chemistry from Lanzhou University of China in 2007. He then moved to Boston University to pursue his Ph.D. in theoretical chemistry with David Coker. Frank's Ph.D. work focused on developing efficient and accurate non-adiabatic dynamic methods to understand the excitation energy transfer process and the electronic coherence in natural light harvesting systems. In 2012 he joined CalTech as a postdoctoral researcher in the group of Tom Miller where he worked on extending the linearized path-integral method to simulate the electron and excitation transfer dynamics, as well as applying a variety of novel computational methods such as ab-initio molecular dynamics tools and wavefunction-in-DFT embedding approach to explore the fundamental aspects of electron and proton transfer mechanisms in cobalt-based hydrogen evolution catalysts. He was recognized as one of the "top reviewers for *The Journal of Chemical Physics*" (2012) and received an "ACS PHYS Division Postdoctoral Research Award" (2014).

The Huo research group develops and applies multi-scale theoretical approaches that combine novel dynamics and methods and scalable electronic structure methods to investigate the complex reaction dynamics associated with solar energy harvesting and storage processes. In particular, the primary research interests focus on: excitation-induced charge separation dynamics in organic photovoltaic devices; photo-induced proton-coupled electron transfer reaction; catalytic fuel generation reactions such as hydrogen evolution.

Frank is also excited about teaching Computational Chemistry (CHM 459), which will focus on the theoretical foundation of computational techniques as well as practical applications in research problems.

## Selected Publications:

Communication: Predictive partial linearized path integral simulation of condensed phase electron transfer dynamics. P. Huo; T.F. Miller; D.F. Coker, *J. Chem. Phys.*, **2013**, *139*, 151103.

Electronic Coherence and the Kinetics of Inter-Complex Energy Transfer in Light-Harvesting Systems. P. Huo; T.F. Miller, *Phys. Chem. Chem. Phys.*, **2015**, DOI: 10.1039, C5CP02517F.

Influence of Environment Induced Correlated Fluctuations in Electronic Coupling on Coherent Excitation Energy Transfer Dynamics in Model Photosynthetic Systems. P. Huo and D. F. Coker, *J. Chem. Phys.*, **2012**, *136*, 115102.

Efficient Energy Transfer in Light-Harvesting Systems, III: The Influence of the Eighth Bacteriochlorophyll on the Dynamics and Efficiency in FMO. J. Moix; J. Wu; P. Huo; D. F. Coker; J. Cao, *J. Chem. Phys.*, **2011**, *2*, 3045.

Communication: Partial Linearized Density Matrix Dynamics for Dissipative, Non-Adiabatic Quantum Evolution. P. Huo and D. F. Coker, *J. Chem. Phys.*, **2011**, *135*, 201101.

Theoretical Study of Coherent Exciton Transfer in Cryptophyte Phycocyanin 645 at Physiological Temperature. P. Huo and D. F. Coker, *J. Chem. Phys.*, **2011**, *2*, 825.

## Robert K. Boeckman, Jr.

Marshall D. Gates, Jr. Professor of Chemistry

Ph.D. 1971, Brandeis University



### RESEARCH INTERESTS

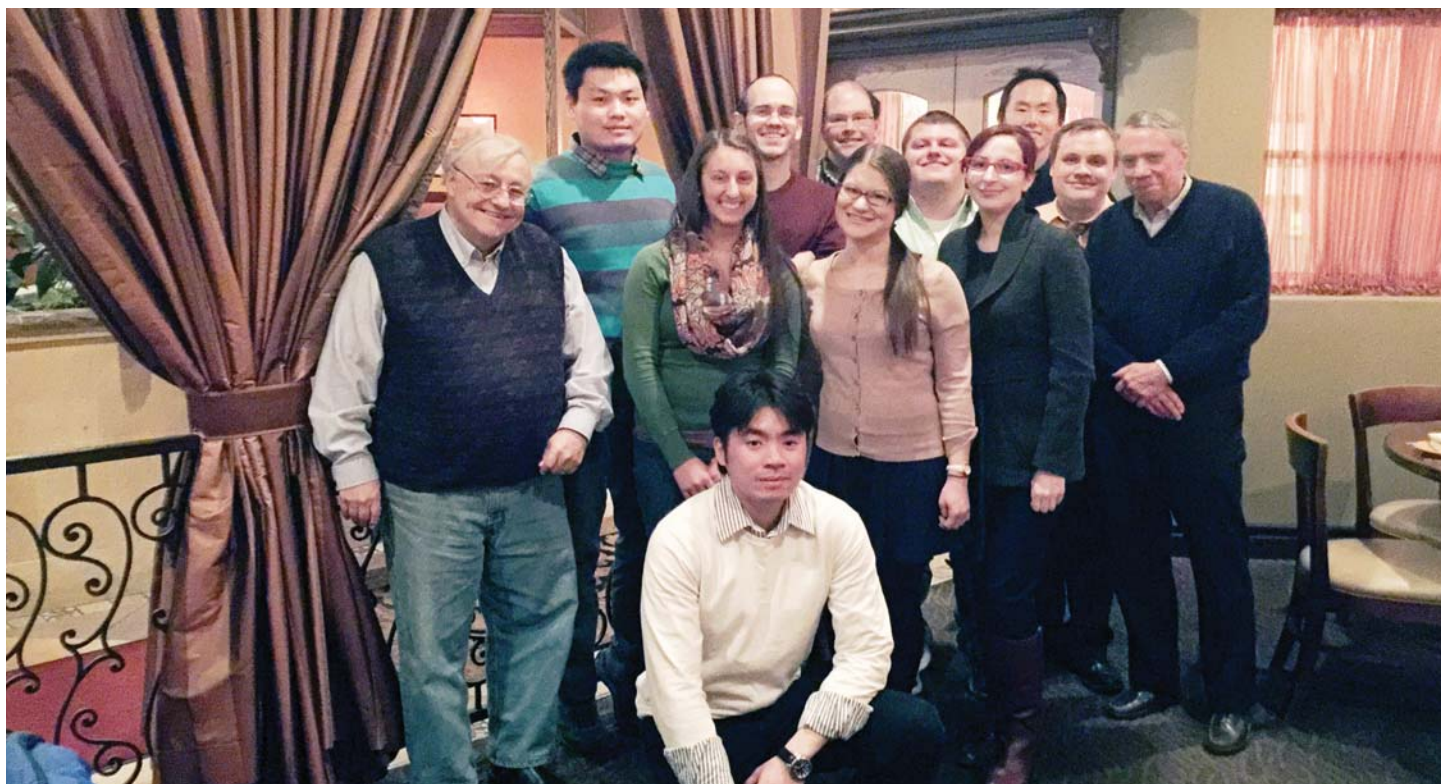
Total synthesis of alkaloids, terpenes, antibiotics, and antitumor agents; development of new synthetic methodology including the asymmetric synthesis methods involving the Diels-Alder reaction, the Claisen-retro-Claisen and other reactions; applications of conformational theory to the development of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

### CONTACT

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During the 2014-2015 academic year **ROBERT K. BOECKMAN, JR.** returned to full time teaching and research following his sabbatical leave. He continues his duties as Associate Editor of the *Journal of Organic Chemistry*, and President and Chair of the Board of Directors of Organic Syntheses, Inc.

The Boeckman 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 the synthesis of FK-506, as well as projects directed toward Apoptolidin. New aza-[3,3]-sigmatropic rearrangement methodology has been developed, which has now been published, and attention is now focused on application of this chemistry to the antitumor Manzamine class alkaloid Nakadomarin A. Work is continuing toward an asymmetric variant of a shelf-stable chromium(III) complex that serves as a precatalyst for Nozaki-Hiyama and Takai



The Boeckman Group (left to right): back row: Hui Wang, Doug Tusch, Kyle Rugg, Kyle Biegasiewicz, Taketo Taguchi, Daniel Austin, Dennis Savage; second row: Bob Boeckman, Heidi Schlager, Taylor Sodano, Sarah Paulson; front row: Lifeng Xiao

type chromium-mediated allylations of aldehydes and for a wide variety of chromium(II) mediated reactions, and additionally on asymmetric vinylogous Mukaiyama aldol reactions catalyzed by chiral oxazaborolidines. The group has also completed their first efforts in organocatalysis with the development of catalytic systems for hydroxymethylation of aldehydes. Studies in this area are continuing toward asymmetric oxidation of aldehydes and other applications. Collaborations continue with **DR. DAMIAN KRYSAN** of the Department of Pediatrics, URM, whose goals are 1) the identification of the biological target(s) of a novel series of small molecules which mimic the effects of caloric restriction on lifespan in yeast and in small mammals, and 2) the development of inhibitors showing specificity for fungal enzymes for use in antifungal therapy against invasive fungal infections of neonates and young infants. Exciting new collaborations between the group, **DR. HAL EBETINO (Ph.D. '84)** (Research Professor in Chemistry) and **DRS. BRENDAN BOYCE** and **LIANPING XING** of the URM Department of Pathology and Laboratory Medicine have been established which have resulted in the development of a Bone Targeted Drug Delivery Platform Technology including promising leads toward Bone Targeted Therapies for Bone Related Effects of Rheumatoid Arthritis, Osteoarthritis and Bone Cancer Chemotherapies.

**GEORGE ARAB (Ph.D. '13)** joined a small biotechnology company **Micromidas** in Sacramento CA working on catalytic biomass conversion to plastics intermediates. **MATT BETUSH (Ph.D. '15)** defended his thesis in August 2015 and continues as a Temporary Visiting Assistant Professor of Chemistry on the faculty of Allegheny College. **SARAH PAULSON (Ph.D. '15)** and **HUI WANG (Ph.D. '15)** defended their theses in the Spring/Summer. Hui completed the total synthesis of (-)-Nakadomarin A. Sarah is currently doing adjunct teaching at RIT while she seeks a research position in the Rochester area. Hui Wang is currently doing post-doctoral work with Dr. Robert DeVita at the Mt. Sinai Medical School in New York City. Fifth year students **DOUGLAS TUSCH** and **KYLE BIEGASIEWICZ** have completed their doctoral requirements and are focused solely on research. Doug is working on the Apoptolidin project, with assistance of third year student **LIFENG XIAO**, and Kyle Biegasiewicz has taken on FK-506 with the assistance of new first year graduate student **JUSTIN NIZIOL (RIT/B.S.)**. **KYLE RUGG (RIT B.S./M.S.)** and **HEIDI SCHLAGER (Wells College/B.A.)** joined the group in January 2014. Kyle Rugg is working on a more refined route to Nakadomarin A, and Heidi Schlager is continuing Matt Betush's work on catalysis including asymmetric versions using Chromium(II) and Copper (I). **DANIEL AUSTIN (Fredonia/B.S. - D.Pharm/SJF)** is working collaboratively with **DR. DENNIS SAVAGE** and Damian Krysan of the URM on a novel antifungal drug candidate to potentially treat *candida cryptococcus* and other fungal infections. Dr. Dennis Savage, retired from Kodak, continues his work in the group on several projects with the Krysan groups (Pediatrics URM).



The Boeckman Group celebrates the wedding of Stephanie Dorn (Weix Group) and Kyle Rugg (Boeckman Group)

# Kara L. Bren

Professor of Chemistry

Ph.D. 1996, California Institute of Technology



## RESEARCH INTERESTS

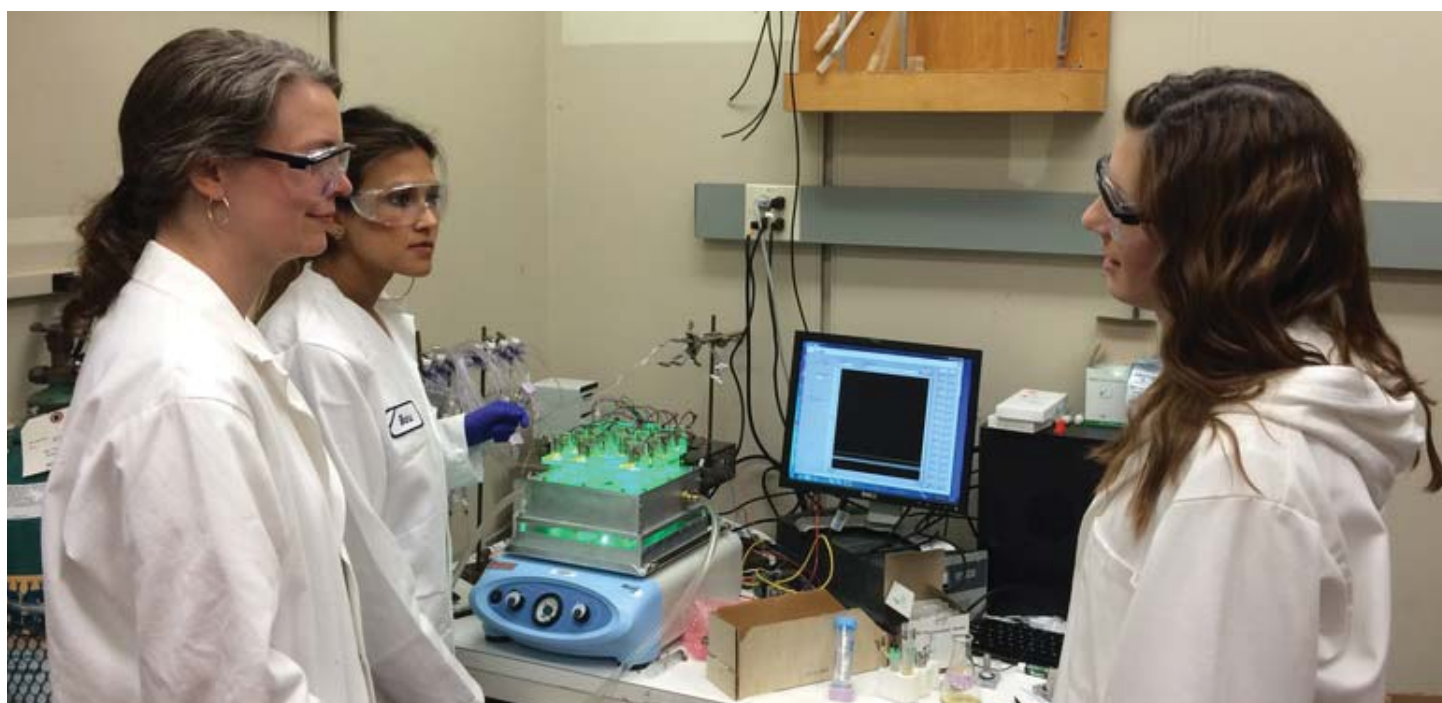
Bioinorganic and biophysical chemistry: engineered metalloprotein and metallopeptide catalysis for solar fuels, biological and nanotechnological systems for solar energy conversion, heme protein structure and function, protein dynamics.

## CONTACT

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**KARA BREN** and her group have been expanding their work in engineering biological systems for solar energy conversion and storage. The Bren group also has been furthering their magnetic resonance studies of metalloporphyrins, with new applications in magnetic resonance imaging. Joining these efforts this year were two researchers. Postdoctoral fellow **DR. PETER LAMBERG** from Malmö University, Sweden is developing biological electron donors for systems for photochemical energy storage. The group's other new member is graduate student **YIXING GUO**, from Portland State University and Sichuan University, who is preparing and studying new metallopeptide electrocatalysts for proton reduction and for nitrite reduction. The group also saw two graduations. Graduate student **LENORE KUBIE (Ph.D. '15)** will be a postdoctoral researcher with Bruce Parkinson at the University of Wyoming, and senior thesis student **LAUREN WEBER (B.S. '15)** was happy to accept a position at Bausch & Lomb doing sample processing and research in their contact lens division.

Peter is collaborating with graduate student **REBECCA SMITH** and with **DR. SANELA LAMPA-PASTIRK** of the Krauss group on the biological electron donor project. This effort is getting the group deeper into bioelectrochemistry and microbiology as we work to identify a sustainable supply of electrons for photochemically driven hydrogen evolution from water. Aiding the work this summer is undergraduate **KATHRYN PROE** (Nazareth College). On the catalysis side of this project are graduate students **SAIKAT CHAKRABORTY** and **BANU KANDEMIR**, who along with Yixing are developing engineered biocatalysts for proton reduction. Saikat is incorporating metal ions into proteins to form novel catalytic sites, and Banu is reengineering cytochromes into artificial hydrogenases. Saikat also is



*Kara Bren, Banu Kandemir, and Rebecca Smith next to the photochemistry apparatus used for photochemical hydrogen generation.*

working to pair catalysts with photosensitizers and has demonstrated that these biological catalysts can be photochemically activated to evolve hydrogen, thus storing light energy as a fuel. Undergraduate **MARISA GUERIN** also has been working on this effort and will continue next year for her senior thesis research. For summer 2015, undergraduates **MANJISTHA MUKHERJEE** (Indian Association for the Cultivation of Science) and **AMIE SANKOH** (RIT) are working with Banu and Saikat over the summer on protein electrochemistry and photochemistry. The group is also continuing its ongoing collaborations with a number of groups including the Lehnert group at the University of Michigan and the Elliott group at Boston University. Also, Rebecca is continuing her collaboration with Xiao-an Zhang's group in Toronto in developing low-toxicity manganese-based MRI agents that show better performance at high field than gadolinium compounds.

Kara kept busy continuing her role as an Associate Editor for the *Journal of the American Chemical Society*, aided by Valerie Drake, who has been the key to an efficient operation. Kara also enjoyed continuing her role in leading the Biological Chemistry Cluster. The successful retreat in May featured talks by Prof. Cynthia Burrows (University of Utah) and Bren group graduate **JASON KELLOGG (Ph.D. '05)** (Siemens Healthcare Diagnostics). We received great news from the Bren group graduates **LEA VACCA MICHEL (Ph.D. '07)** (RIT, Department of Chemistry) and **AMY ENSIGN KOVACH (Ph.D. '09)** (Roberts Wesleyan College, Department of Chemistry); both were promoted and received tenure this year. Kara also kept a busy travel schedule. Highlights included speaking in the inaugural Harry Gray Award Symposium at the ACS National Meeting in Denver, CO and participating in a workshop on hydrogenase mimics in Telluride, CO.



*The Bren Group 2015 (left to right, from top): Kara Bren, Peter Lamberg, Saikat Chakraborty, Banu Kandemir, Rebecca Smith, Yixing Guo, Kathryn Proe, Manjistha Mukherjee*

# Joseph P. Dinnocenzo

Professor of Chemistry

Ph.D. 1983, Cornell University



## RESEARCH INTERESTS

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

## CONTACT

jpd@chem.rochester.edu

**JOE DINNOCENZO** and his group continue to pursue a variety of problems in electron transfer and related chemistry. The projects include investigating interesting cation radical reactivity, unusual exciplex intermediates (in collaboration with Samir Farid and Ralph Young), and a novel reaction between alkoxy radicals and pyridine bases in which a hydrogen atom is transferred from the alkoxy radical to the pyridine base (also a collaboration with Samir Farid).



PLTL Lunch before Meliora Weekend (left to right): Todd Krauss, Adam Feinberg, Ben Hafensteiner, Elliot Richman, Jared Kneebone, Nick Hammond, Terrell Samoriski.

undergo fragmentation to preferentially give the less stable aryl radical rather than a methyl radical. Adam is currently working to fully understand the mechanism of these reactions. Over the past year Adam gave talks on his research at both the 2015 Physical Organic Gordon Research Conference and the ACS meeting in Boston.

**TERRELL SAMORISKI** completed her Ph.D. research project on the design, implementation, and evaluation of the Peer Led Teaming Learning (aka Workshops) model in the undergraduate organic laboratory, specifically our Honors Organic Laboratory II (CHM 210). Along with other findings, Terrell's research has shown that students find Workshops help them to be better prepared for lab and assists them with their data analysis – two perennial problems experienced in laboratory courses. Terrell is the first graduate student in the history of the Rochester chemistry department whose Ph.D. project was in the area of chemical education.

The Dinnocenzo group welcomed **ANALUZ MARK**, a first-year graduate student, to the group over the past year. Ana's research efforts are currently focused on novel fragmentation reactions of Group 14 cation radicals.

Graduate student **ADAM FEINBERG** has recently used nanosecond transient absorption spectroscopy to provide direct experimental evidence that alkoxy radicals can react with pyridine bases to give pyridinyl radicals. As far as we are aware, these are the first examples of alkoxy radicals acting as hydrogen atom donors in their reactions with a closed shell molecule. Adam is also working to understand the general mechanism for fragmentation of aryltrialkyl Group 14 cation radicals. Adam has discovered that like aryltrimethylstannane cation radicals (previously investigated in the group by **PU LUO (Ph.D. '12)**, aryltrimethyl-silane and -germane cation radicals



Adam Feinberg and Analuz Mark



# Richard Eisenberg

Professor of Chemistry / Research Professor

Ph.D. 1967, Columbia University



## RESEARCH INTERESTS

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

## CONTACT

eisenberg@chem.rochester.edu

While wonderful events and occasions happened for **RICH EISENBERG** this past year, the period also marked the start of a general transition for his laboratory. Specifically, the last of Rich's formally advised graduate students, **RANDY SABATINI (Ph.D. '15)**, who worked jointly with Dave McCamant, received his Ph.D. and has moved on to a postdoc position at the University of Toronto, while postdocs **AMIT DAS, PURNIMA RUBERU** and **BO ZHENG** also completed their appointments and are off to future career challenges. The reduction in group size has also led to an ongoing reconfiguration and consolidation of Rich's lab space. This is the most significant change in lab space that Rich has experienced in more than 40 years at Rochester, so it comes with lots of memories, as well as dealing with notebooks, spectra and samples from legions of students and postdocs over the years (the samples were all disposed in accordance with approved procedures, as Ken Simolo will attest). That said, the Eisenberg lab is not closing-it is getting smaller, reorganized, and refurbished. In July 2015, Rich, along with colleagues Kara Bren and Todd Krauss, received a three-year \$1.05 million grant from the Department of Energy Office of Basic Energy Sciences to continue their work on the reductive side of solar-driven water splitting and the generation of hydrogen from aqueous protons (plus, of course, electrons). Rich anticipates that in September the group will have two postdocs working on the project, along with a possible undergraduate or two.

The publications of the past year document continued progress in Rich's focus on solar hydrogen and include efforts to make more effective light absorbers by coupling strongly absorbing organic dyes to charge-transfer metal complex chromophores for enhancement of photoinduced electron transfer, and the first studies within the group on new photocathodes in order to eliminate the need for sacrificial electron donors in light-driven H<sub>2</sub> generation.



*Rich with Kara Bren, and former UR faculty members Shaul Mukamel and Dwayne Miller*



Rich and Harry Gray at the March 2015 ACS meeting in Denver

In September 2014, Rich gave the Russell Marker Lecture at Penn State University and received the John C. Bailar, Jr. Award at the University of Illinois in Champagne-Urbana. The latter was particularly meaningful because of Bailar's great influence on inorganic chemistry in the U.S. and the fact that he is a "chemical forefather" of Rich (Bailar-Basolo-Gray-Eisenberg). In October, Rich traveled to Sapporo, Japan to deliver a special lecture at their Annual Meeting on Photochemistry. He was hosted by Dr. Atsushi Kobayashi who had visited Rich's lab for six months in 2012. In March 2015, Rich was at the ACS Meeting in Denver to speak in several symposia and mark several special occasions. One was to honor his good friend Maurice Brookhart of UNC who won the Gabor Somerjai Award in catalysis, the second was to help Kim Dunbar celebrate the ACS Distinguished Service in Inorganic Chemistry Award (in addition to being a friend, Kim is an *Inorganic Chemistry* Associate Editor originally appointed by Rich), and the

third was to celebrate the first Harry Gray Award for Creative Research by a Young Investigator in Organic Chemistry. The last was truly special since Rich has led the effort to inaugurate this award in honor of Harry, his friend and mentor for more than 50 years, who will turn 80 in 2015. The new award, and the successful efforts to endow it, received special recognition at the awards dinner and ceremony from Dr. Pat Confalone, the ACS Chair of the Board.



On the personal side were travels to New Zealand with Marcia for much of February, exploring both north and south islands. The country is beautiful and the scenery, especially on the South Island, is spectacular with glaciers, snow-covered mountains, rainforests, and far too many sheep to count, even with the most severe insomnia. In May, Rich traveled to Houston where son Alan did an Ironman 140.6—an astonishing accomplishment under any circumstances, but even more so in light of several earlier knee surgeries. Plans are being set in motion for an eventful 2015-16, as well as for Marcia and Rich's annual snow-bird migration to Sarasota, Florida.



## RESEARCH INTERESTS

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

## CONTACT

farid@chem.rochester.edu

**SAMIR FARID'S** research continues to be on photochemistry and the photophysics of electron transfer processes, in collaboration with Joe Dinnocenzo and Ralph Young. Our previous work on the effect of strong mixing on exciplex emissions and the role of varying degrees of charge transfer character was extended to the effect of solvent polarity on the degree of stabilization of the ion pair. Surprisingly, small changes in the structure of the donor or the acceptor have profound effect on the degree of stabilization of ion pairs. In low polarity solvents radical ion pairs ( $A^{\bullet-}D^{\bullet+}$ ) of equal redox energies are more stabilized when the acceptor is harder to reduce (more negative reduction potential) or the donor is harder to oxidize (more positive oxidation potential). That difference decreases with increasing solvent polarity and is absent in highly polar media – as the solvent stabilization becomes more important than the coulombic attraction.

*Rush Rhees in the snow (Longze Zhang)*



# James M. Farrar

Professor of Chemistry

Ph.D. 1974, University of Chicago



## RESEARCH INTERESTS

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

## CONTACT

farrar@chem.rochester.edu

Imaging ion-molecule reactions continues as the theme for **JIM FARRAR** and his research group. Over the past year, our work has focused not only on reactions of importance in astrochemistry – hence our reputation for being “Lost in Space” – but also on the reactions of gas phase ions with free radicals. This has been a pretty good year for radical chemistry. We have finally managed to coax reasonable concentrations of methyl and allyl radicals from the silicon carbide afterburner source that Barney Ellison (University of Colorado) convinced us to use, and published our first paper on the subject. Owing to a generous reviewer of this paper, Jim was invited to present a talk at the 33<sup>rd</sup> International Conference on Free Radicals at Squaw Valley, California this summer.

The group continues to enjoy collaborations with scientists from all over the world. Last summer, we welcomed **EDUARDO CARRASCOSA**, a native of Madrid, who is studying for his Ph.D. degree in the research group of Professor Roland Wester at the Institute for Ion Physics of the University of Innsbruck. Eduardo stimulated us in many dimensions, from the way in which we conduct our experiments to the details of our data analysis. He challenged us to be sure we got the mass spectrometry right, and that was essential for our radical chemistry work. We also continued our forty-year long collaboration with Molecular Beam group in Perugia as Jim traveled to the “Elletre” synchrotron light source in Trieste for a series of experiments on multiply-charged molecular cations. It was very interesting to see how science is done at a national facility. Jim also enjoyed having two very talented undergraduates in the lab. **NAN YANG (B.S. '15)** did his senior thesis in the group, the results of which led to significant improvements in the optical design of our imaging system. Nan will enter Yale’s Ph.D. program this fall. **PING HE (B.S. '16)** also joined the group, first as an REU student, and now as a senior thesis student. She has already made important contributions with her theoretical work on reactive intermediates in ion-radical chemistry, and will continue both her experimental and computational work during the academic year.

After several years of teaching quantum chemistry to juniors and seniors during the Fall semester, Jim has switched his emphasis to teaching a one-semester course in general chemistry for engineers. It will be interesting to see how emphasizing “the rules” of chemistry and solving problems with those rules will work out.

Jim and Kathy continue to enjoy their roles as grandparents, without a doubt “the best gig in the world.” Grandsons Callum and Cary live in Manhattan with parents Stacey and Achim, and granddaughter Josefina (“Fi-Fi”) and her parents, Mariana and Andy, have moved to Amherst, Massachusetts, as Mari began a faculty position in Neuroscience at the University of Massachusetts in September of 2014.



Jim's grandchildren, Fi-Fi, Callum, Cary



## RESEARCH INTERESTS

Bioorganic chemistry, biocatalysis, and chemical biology; synthesis and directed evolution of macrocyclic peptides as modulators of protein-protein interactions; chemoenzymatic synthesis; design and engineering of metalloprotein catalysts for C-H functionalization and carbon-carbon and carbon-heteroatom bond formation.

## CONTACT

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Professor **RUDI FASAN** and his group continue to investigate the development of novel chemobiosynthetic methodologies for the synthesis and evolution of peptide-based macrocycles as inhibitors of protein-protein interactions and the design and application of metalloprotein catalysts for synthetic applications. A number of important accomplishments were made over the past year in the area of macrocyclic peptides. A first one involved the development of a method to achieve the spontaneous, post-translational cyclization of ribosomal peptides in bacterial cells. This project, which was conducted by graduate students **JOHN FROST (Ph.D. '15)** and **ANDREW OWENS** with the assistance of former undergraduates **LOUIS PAPA (B.S. '14)** (currently a grad student at MIT) and **NICK JACOB (B.S. '13)** (currently a grad student at Scripps La Jolla), has yielded a new strategy to construct libraries of side-chain-to-tail macrocyclic peptides in bacteria, which could be readily applied to identify cyclopeptide inhibitors of a model target protein (*ACS Chem. Biol.* 2015). Taking inspiration from the biosynthetic logic of certain classes of naturally occurring cyclopeptides such as lanthipeptides, postdoctoral fellow **NINA BIONDA** and former student **ABBY CRYAN (M.S. '14)** (now at Modern Industries) implemented a methodology to enable the ribosomal synthesis of conformationally constrained peptides carrying an inter-side-chain thioether bond (*ACS Chem. Biol.* 2015). The scope of this peptide macrocyclization strategy could be later extended to provide access to 'natural product-like' bicyclic peptides and this approach could be applied to develop high affinity binders of streptavidin (*ChemBioChem* 2015). John successfully defended his Ph.D. thesis in the Fall of 2014 and soon thereafter joined the Yudin group at the University of Toronto as a postdoctoral fellow. Along with John, we bid a fond farewell also to Nina who moved on to acquire a Senior Research Scientist position at iFyber, an Ithaca-based company specialized in the manufacture of biomedical devices. Our program on peptide macrocycles is now led by third-year graduate student **ANDREW OWENS** and **PHUONG THUC NGUYEN**, a new postdoc from the Nanyang Technological University in Singapore, who are investigating the potential of our macrocyclic peptide scaffolds toward disrupting key protein-protein interactions involved in cell signaling pathways misregulated in cancer and other diseases.

Our subgroups working in the area of metalloprotein catalysis have also reported major accomplishments this past year. Postdoctoral researchers **VIKAS TYAGI** and **SIMONE GIOVANI**, who recently joined our group from the University of Siena in Italy, have developed novel chemoenzymatic routes based on late-stage P450-mediated C-H oxyfunctionalization to obtain improved analogs of naturally occurring sesquiterpene lactones with antileukemic activity. Second-year graduate student **HANAN ALWASEEM** is currently investigating the mechanism of action of these compounds and their biological activity across other types of cancer. In a paper published in *ACS Catalysis*, postdoctoral fellow **RITESH SINGH** and **JOSHUA KOLEV (Ph.D. '15)** have expanded the reaction scope of engineered P450 enzymes to promote the intramolecular C(sp<sup>3</sup>)-H amination of carbonazidates to give oxazolidinones. While this study also provided initial insights into the nature of the C-H activation step of P450-catalyzed C-H amination, the mechanistic aspects of this novel class of biocatalytic reactions are currently being investigated by **TESSA WOODRUFF**, who became part of our lab as a joint student with the Neidig group. With the technical assistance of undergraduate students **RACHEL BONN** and **EDGAR ALANIZ**, a fearless team consisting of **DR. VIKAS TYAGI**, **DR. GOPEEKRISHNAN SREENILAYAM**, and **DR. MELANIE BORDEAUX**, has contributed to make major inroads in the development of hemoprotein-based catalysts for carbene transfer reactions. Specifically, we discovered that the heme-containing protein myoglobin can furnish a promising and robust scaffold for the development of highly

efficient and selective biocatalysts for the cyclopropanation of aryl-substituted olefins (*Angew. Chem. Int. Ed.* 2015) and the formation of C–N and C–S bonds via the insertion of carbenoid species into N–H (*Chem. Commun.* 2015) and S–H bonds (*Chem. Sci.* 2015), respectively. These studies, which have been highlighted in various journals including *Nature Chemistry*, have opened an entirely new area of research in our laboratory. The team, which has recently been joined by **DR. PRIYANKA BAJAJ** from the National Institute of Pharmaceutical Education and Research in Mohali, India, is currently exploring the scope of myoglobin-derived catalysts across a variety of other synthetically valuable transformations.

In addition to those mentioned earlier, other members of the group have moved on to new positions in academia or industry. After defending his Ph.D. thesis in August of 2015, Josh joined the Biocatalysis Process Group at Merck as Senior Scientist, whereas Melanie and Ritesh moved to the Louisiana State University Medical School and to the Ulsan National Institute of Science and Technology in Korea, respectively, for a second postdoctoral experience. Last year, four talented undergraduates completed their Senior Thesis Research in our lab and graduated amidst a number of accolades for their research and academic accomplishments: **NICHOLAS HILL (B.S. '15)**, who will pursue a Ph.D. at the University of Colorado at Boulder, **ZHIJIE (ABE) WU (B.S. '15)**, who will join the chemistry graduate program at the University of Wisconsin-Madison, **QI YING (QUEENIE) LI (B.S. '15)**, who will be a MD candidate at the Albert Einstein Medical School in NYC, and **JOHN DECOURCEY (B.A. '15)**, who will join a biotech company in the Boston area. As we wish best of luck to the former group members for a bright future and career, we send our heartiest congratulations to **TESSA WOODRUFF** for the award of a National Science Foundation Graduate Fellowship, to undergraduate student **CHRISTINE ZIEGLER** for receiving the Catherine Block Memorial Fund Prize, and to former students Nick Hill and Abe Wu for being selected to present their research at the 2015 National Conference for Undergraduate Research in Cheney, WA. Congratulations also go to former graduate student **JESSICA SMITH (Ph.D. '14)**, who has landed an academic position at SUNY Brockport.

The past year has involved a rather hectic traveling schedule for Rudi, who had the opportunity to share the results of his group as part of invited lectures in various conferences across the country and abroad. These events included the Breslow Award Symposium at the 249th ACS National Meeting in Denver, the 3rd Macrocyclics and Constrained Peptide Conference in San Diego, the 19th International Conference on Cytochrome P450 in Tokyo, the 12th International Symposium on Cytochrome P450 Biodiversity and Biotechnology in Kyoto, and the 15th Tetrahedron Symposium-Asian Edition in Singapore. At home, Rudi and Francesca continue to enjoy the little moments of serenity and happiness their daughters Penelope (3.5 year old) and Maia (2 year old) give them every day.



*The Fasan Group (left to right): 1st row: Queenie Li, Katherine Grasso, John Frost, Melanie Bordeaux, Garrick Centola; 2nd row: Rudi Fasan, Hanan Alwaseem, Tessa Woodruff, Christine Ziegler, Gopeekrishnan Sreenilayam; 3rd row: Ritesh Singh, Abe Wu, Nina Bionda, Rachel Bonn, Edgar Alaniz, Nick Hill; 4th row: Vikas Tyagi, Francesca Vitali, Shaun Ben-ari, Andrew Owens, Joshua Kolev*

# Ignacio Franco

Assistant Professor of Chemistry

Ph.D. 2007, University of Toronto



## RESEARCH INTERESTS

Laser control of electronic properties and dynamics, electronic decoherence in molecules, theory and simulation of single-molecule pulling processes, novel spectroscopies and control in single-molecule junctions.

## CONTACT

franco@chem.rochester.edu

The second year of the **FRANCO** group has been hectic and exciting. As our young group matures, so does our ability to tackle problems at the frontier of knowledge in Chemistry, Physics, Optics, and Nanoscience. Through theory and simulation, we continue to investigate general problems in Chemistry and, in particular, the problem of how to control electrons using lasers and how to control molecules in junctions.

In a recently published paper, postdoc **DR. LIPING CHEN** demonstrated how to model time-dependent transport processes in junctions through an accurate and extremely simple method. She is also in the final stages of a simulation tour de force to explain what is currently the fastest existing method for the generation of currents in nanojunctions. At a personal level, Liping and her husband **DR. LINJUN WANG** had their first daughter, **MENGDIAN**, born in the fall of 2014. Postdoc **DR. ARNAB KAR** has continued his bold transition from High-Energy Physics into Chemistry. In our group, he has been teaching us math, daring us into squash matches, and investigating fundamental aspects of electronic decoherence in molecules. Some of his results are currently being considered for publication. The two Ph.D. students in the group, **ZHI LI** and **RACHEL CAREY**, have now completed their cumulative exams, courses, and qualifying exams, and are now officially Ph.D. candidates. As molecular-torturers-in-training, Zhi and Rachel investigate how to model single-molecules sandwiched between electrodes, and how to probe and control chemistry in this setting through applied voltages and forces. This year, we also had undergraduates **ULISES HERRERA** and **LEOPOLDO MEJÍA** from Mexico and Colombia, respectively, doing research during the summer in the group.

In addition to doing research and writing grants, Ignacio was a member of the Faculty and Graduate Recruiting Committees, and lead the creation of a new program to bring top international graduate students to do research during the summer in the Department. Ignacio also taught graduate Quantum Mechanics (CHM 451) in Fall 2014 for the second time, and Statistical Mechanics (CHM 455) in Spring 2015 for the first time.

This academic year was full of travel and presentations for our group members. Ignacio gave talks in New York, Vancouver, Medellin, APS San Antonio, Berlin, Hamburg, Copenhagen, Lake Garda and Telluride. Additionally, Ignacio and Arnab participated in the Gordon Conference on Quantum Control. Rachel attended the Telluride Summer School in Theoretical Chemistry and gave a presentation to roughly 800 high school students during the New York State Science Olympiad competition at Le Moyne College. In June, the group ventured into the Laboratory of Laser Energetics for a tour with Dr. Dan Haberberger as a host. In addition to our travels, we had the pleasure of hosting several visitors during the school year including Angel Rubio, Valeria Molinero, Alex Tkatchenko, Neepa Maitra, Sergei Tretiak, Mark Tuckerman and Adrián Roitberg.

We look forward to a successful new year of research, teaching and service.



*The Franco Group (left to right): Arnab Kar, Lijun Wang, Zhi Li, Ignacio Franco, Rachel Carey, Ulises Herrera, Leopoldo Mejia, Liping Chen*

# Alison J. Frontier

Professor of Chemistry

Ph.D. 1999, Columbia University



## RESEARCH INTERESTS

Synthetic organic chemistry; synthesis of bioactive natural products; pericyclic reactions; asymmetric catalysis; cationic cascades.

## CONTACT

frontier@chem.rochester.edu

Professor **ALISON FRONTIER'S** research program is devoted to synthetic organic chemistry. Research directions being pursued in the lab include the study of novel pericyclic reactions, cationic rearrangements and stereoselective cyclization cascades, and their application to complex molecule synthesis. Projects focus on reactions that can produce unusual, densely functionalized ring systems from simple precursors for rapid assembly of polycyclic structures found in rare natural products. The lab has identified several variants of the Nazarov cyclization since studies began in 2002, making it possible to synthesize highly substituted cyclopentanes with different substitution patterns. Continuing the work of **JOSHUA BROOKS (Ph.D. '12)**, and **STEVEN JACOB (Ph.D. '15)**, **YU-WEN HUANG** developed an enantioselective version of the 4p (Nazarov) electrocyclization initiated by 1,6 conjugate addition to dienyl diketones. Yu-Wen has also discovered a new cyclization cascade that assembles complex bridged bicyclic ring systems in a single step, from simple dienyl diketone precursors. Our ongoing collaboration with Rich Eisenberg has become focused on a novel type of heterogeneous gold catalyst and its Lewis acidic reaction chemistry. New studies of cationic cyclization cascades strengthen our conviction that the gold complex offers exciting alternative reactivity compared to conventional Lewis acids. Studies targeting bioactive natural products continue, with projects targeting tetrapetalones, tubingensins, arnicenone and related triquinanes, and elisabanolide.

We welcomed **DR. CORINNE MINARD** (from Institut de Chimie des Substances Naturelles, Gif sur Yvette, France), a Ph.D. student of group alumnus **KEVIN CARIOU (FLW'09)**, to the group. She is studying novel Lewis acid-catalyzed cationic cyclization sequences. **DYLAN PARSONS** joined the group this year, and his work is focused on cascade cyclizations that build angular fused ring systems, and the application of this method to natural product synthesis. We also congratulate **PETER CARLSEN (Ph.D. '15)** and **STEVEN JACOB (Ph.D. '15)**, who successfully defended their doctoral theses this year. Peter is pursuing postdoctoral studies with Professor Andrew Myers at Harvard University, and Steve is at UC Berkeley, doing postdoctoral research with Professor Dean Toste.



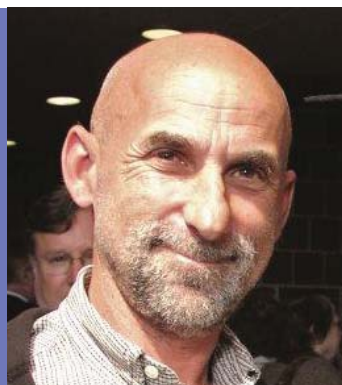
*The Frontier group: 1st row (left to right): Jeremy Cody, Alison Frontier, Corinne Minard, Murray Wan  
2nd row: George Alachouzos, Mike Moscovitz, Dylan Parsons, Pat Harrington, Eric Stoutenberg, Yu-Wen Huang*



## Joshua L. Goodman

Professor of Chemistry

Ph.D. 1984, Yale University



### RESEARCH INTERESTS

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

### CONTACT

goodman@chem.rochester.edu

**JOSH GOODMAN** is currently serving as the Chair of the Undergraduate Studies Committee. His research interests are focused on the investigation of organic reaction mechanisms using a variety of time-resolved techniques such as pico- and nanosecond absorption spectroscopy, and photoacoustic calorimetry. In particular, he has been examining processes in which electron transfer is coupled to bond breaking, and/or bond making.

## William D. Jones

Charles F. Houghton Professor of Chemistry

Ph.D. 1979, California Institute of Technology



### RESEARCH INTERESTS

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

### CONTACT

jones@chem.rochester.edu

The **JONES** group continues to actively pursue organometallic chemistry and catalysis. We had two new postdocs join the group this year, **DR. CASSANDRA HAYES** and **DR. SARINA BELLOWS**. Cassandra will be working on a joint project with Tom Baker at U. Ottawa, and Sarina will be working jointly with Tom Cundari at Univ. North Texas. **DR. SUMIT CHAKRABORTY** is continuing as a postdoc, but will leave later this fall to take a new position at Tennessee Eastman. We have also had a visiting professor for the past year from Huaihai Institute of Technology, **DR. RUI-BO XU**. With 3 undergraduate REU students for the summer, the lab is full with 13 people. Our research is examining the activation of C-H bonds in substituted hydrocarbons, C-S cleavage and functionalization reactions of thiophenes, and the acceptorless dehydrogenation of amines and alcohols. An important advance this year has been the discovery of a new process for converting ethanol to n-butanol in a highly selective fashion. The group continues its role in the Center for Enabling New Technologies through Catalysis (CENTC), in which the group has collaborative research projects that are exploring new electrophilic C-H activation catalysts, new direct routes to aniline from benzene, and the above mentioned butanol process. Bill continues as Associate Editor for the *Journal of the American Chemical Society* for a twelfth year, where he handled close to 500 manuscripts last year. He lectured in Heidelberg, Tokyo, Sapporo, Kyoto, Chengdu, Wuhan, and Nanchang, and gave talks at Boston College, Wayne State, at the Denver and San Francisco ACS meetings, and at the DOE Catalysis Conference. He also was the Thursday night lecturer at the 2015 Gordon Conference on Organometallic Chemistry.

The group's scientific accomplishments have centered upon our work in amine and alcohol dehydrogenation, where we established that an iron PNP complex could catalytically dehydrogenate alcohols to ketones without a hydrogen acceptor. Likewise, bicyclic amines could be dehydrogenated to quinolines without an acceptor. The reverse



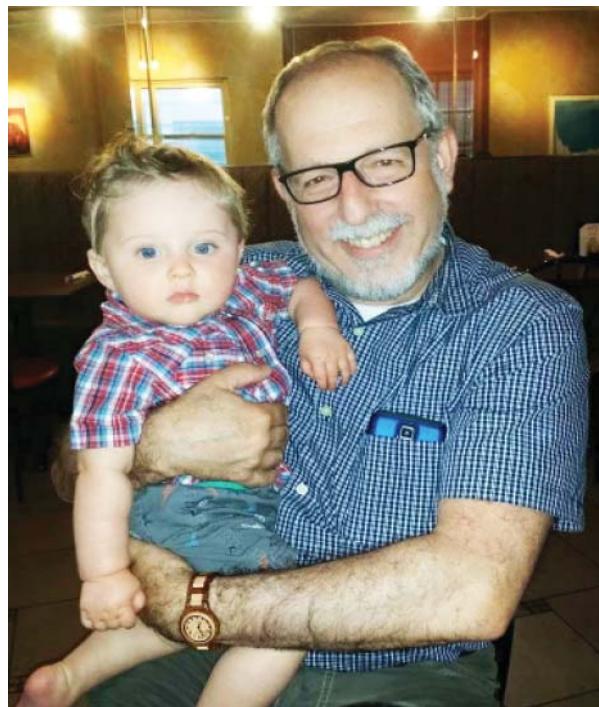
*The Jones group (left to right): Aaron Walsh, Hongmei Yuan, Miles Marnell, Jing Yuwan, Bill Jones, Sarina Bellows, Rui-Bo Xu, Cassandra Hayes, Sumit Chakraborty*

hydrogenations occurred readily under mild conditions. We also completed research with the GE based EFRC Center for Electrocatalysis, Transport Phenomena, and Materials for Innovative Energy Storage. Here we used our catalysts for alcohol dehydrogenation as part of an electrochemical fuel storage project. This work tied in to our recent studies of ethanol condensation to make butanol via the Guerbet process. Here, ethanol is dehydrogenated to acetaldehyde, which then undergoes an Aldol condensation with itself to produce an  $\alpha,\beta$ -unsaturated aldehyde. Rehydrogenation gives butanol, with water as the only byproduct. We have found a very selective tandem catalyst system that yields only n-butanol but no higher Guerbet products (products resulting from butanol reacting in a similar fashion with itself or with ethanol).

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 collaborative research and is beginning its ninth year of phase 2 funding (\$4M/yr). Our group has completed several collaborative projects with the Goldman group, the Brookhart group, and the Cundari group through CENTC, and will continue with 4 new projects this year.

Bill was invited back to China last fall to help teach a course in kinetics to young Chinese professors, and also visit Lushan Mountain, one of the places Mao frequented. He will serve on the International Advisory Board for the ICOMC, ICHA, and OM&Cat conferences. The group is supported by continuing funding from the Department of Energy, the National Science Foundation, and the NSF Center Enabling New Technologies through Catalysis.

On September 10, 2014, Bill became a grandfather with the arrival of his first grandson, Henry William Simson, born to his daughter Sarah and her husband Michael. Henry is thriving, and Heather and Bill are delighted to see him often since they live in Rochester near Sea Breeze in Irondequoit.



*Bill Jones and baby Henry*



## RESEARCH INTERESTS

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

## CONTACT

krauss@chem.rochester.edu

Time for that annual report on the latest and greatest happenings in the **KRAUSS** group!

This past year was our busiest yet with respect to Ph.D. graduations. **FEN QIU (Ph.D. '15)** defended her thesis on the use of semiconductor nanoparticles as robust photosensitizers for the photochemical production of hydrogen. She has since moved to Lawrence Berkeley Laboratory for her postdoctoral position. **CUNMING LIU (Ph.D. '15)** also graduated in late 2014 and moved to the University of Central Florida in Tampa to study more ultrafast photophysics as a postdoctoral fellow. **GREG PILGRIM (Ph.D. '15)** graduated earlier this year, defending a thesis on the use of aligned carbon nanotube membranes as improved materials for simultaneous electron and hole transport over long distances. Greg recently moved to Kyoto, Japan for a postdoctoral fellowship from the Japanese Society for the Promotion of Science. It was very comforting to Greg to know that Thorlabs still delivers lab snacks in Japan! Finally, **HELEN WEI (Ph.D. '15)** also defended her thesis this past summer on using secondary phosphines to control surface stoichiometry for quantum dots. Helen will soon be returning to Taiwan to run the family business. Good luck Drs. Fen, Cumming, Greg and Helen with your future careers!

**KELLY SOWERS** got her first paper published on CdSe quantum dots capped with Cd or S termination, which is quite interesting because the two different surfaces behave quite differently with respect to their fluorescence properties. She is now collaborating with the Bren group on a wild project of generating solar hydrogen with a living system consisting of CdSe quantum dots and electrogenic bacteria, the latter of which provide a natural source of electrons to the CdSe. **AMANDA PRESKE** submitted two papers this year describing tuning the size of PbSe and PbS nanocrystals by changing the ligand attached to the Se or S during the synthesis. She also synthesized an intriguing new quantum dot material in the group, SnSe, and can control the size reproducibly. SnSe QDs are an indirect gap material and so we are collaborating with Sasha Efros from the Naval Research Laboratory to try and understand the shift in quantum dot energy levels with size. This past summer **LEAH FRENETTE** went to several countries in southern Africa as part of the NSF IGERT fellowship program. After she returned to the U.S., Leah finished up mechanistic studies of the CdSe quantum dot reaction mechanism. Leah is going "Back to the Future" as what she found is that the old ways of making quantum dots from the late 1980s are actually what is taking place in the reaction vessel upon breakdown of the "modern" chemical precursors.

**NICOLE BRIGLIO COGAN** spent a lot of the past year studying single molecule color center defects in quartz. These defects interestingly are brightened by a factor of 10 with appropriate chemical treatment, and on the single molecule level show no blinking behavior. We are quite excited to explore the quantum optics implications of this novel and unusual fluorophore. **ZHENTAO HOU** had a major breakthrough with her studies of single carbon nanotube fluorescence at high spatial resolution on the single tube level. She found that very long nanotubes brighten uniformly when certain small molecules are added to the solution. We don't understand it all yet, but the result was so exciting that she won a poster presentation prize at the WONTON 2015 meeting in Germany. Congrats Zhentao! **AMANDA AMORI** has studied the temperature dependence of nanotube photoluminescence for various nanotube structures focusing on a formally forbidden optical transition. From the temperature dependence of the transition Amanda has concluded that intervalley scattering of the exciton in nanotubes causes the transition to be brightened. I expect her paper, which is in progress, will make an important contribution to the nanotube photophysical literature in the next year.

**ABBY FREYER** has successfully doped CdSe quantum dots with silver ions, which makes them either n- or p-type depending on the doping level. She has gotten some great data on the charge properties of the doped quantum dots using electrostatic force microscopy, which is extremely hard to pull off on the single particle level. **JENNIFER URBAN**, our first joint **NILSSON-KRAUSS** student, is attaching peptides onto CdSe quantum dots for the purpose of studying where they bind to neurons with super-resolution microscopy. Jen has some great images that localize the quantum dots to peptide binding sites to within 50 nm, an improvement in resolution of over a factor of 5! Finally, we wanted to welcome our new student **BECKAH BURKE** (nee Johnson) into the group. Beckah is making good progress on highly engineered quantum dots for solar photochemical proton reduction experiments.

**DR. SANELA LAMPA-PASTIRK** joined the group as our research scientist last summer. She is an expert on ultrafast spectroscopy, and in addition to helping organize the chaos of running the group, she is going to measure electron transfer rates from quantum dots to catalysts using the very old, but still working, ti:sapphire regenerative amplifier system.

During the summer the group hosted undergraduates **ANDREW BOYCE** from Boston College, **KEVIN DENNY** from Nazareth College, and **AUSTIN BAILEY** and **CALEB WHITTIER** from the University of Rochester. Austin worked on synthesizing polymers that preferentially solubilize nanotubes of specific chiralities with Amanda Amori. Caleb worked with Amanda Preske on making PbSe quantum dots capped with SrSe, Kevin worked with Leah making CdSe nanoplatelets, and Andrew worked with Sanela coding Lab View to enable us to make PLE maps on the new fluorometer system. Caleb and Austin liked research so much that they will return to work with us during the academic year for independent study.



*The Krauss group (left to right) Fen Qiu, Greg Pilgrim, Nicole Cogan, Leah Frenette, Kelly Sowers, Todd Krauss, Jennifer Urban, Amanda Preske, Amanda Amori, Sanela Lampa-Pastirk, Abby Freyer, Lenore Kubie, Zhentao Hou, Dylan Gaeta, Tianyu Jiao, Cris Vela, Cunming Liu*

# Thomas R. Krugh

Professor of Chemistry

Ph.D. 1969, Pennsylvania State University



## RESEARCH INTERESTS

Biophysical chemistry; structural analysis of biomolecules from two-dimensional NMR, fluorescence, and UV-visible spectroscopies, along with energy minimization and molecular dynamics calculations.

## CONTACT

krugh@chem.rochester.edu

During the past year **TOM KRUGH** continued his support of graduate and undergraduate education. During the spring and summer his main project involves organizing our NSF-supported Research Experience for Undergraduates (REU) program. This summer (2015) we had 31 undergraduates participating in the REU program. 13 students were from other schools along with 18 UR undergraduates. Our REU program reflects support for undergraduate research by faculty, the Chemistry Department, and the College. Undergraduate research provides an opportunity for graduate students (and postdocs) to gain leadership experience through one-on-one mentoring of undergraduates, both in the summer and during the school year. Mentors often describe their experience as important milestones in their graduate career.



Summer 2015 REU Students (left to right, front to back):

1st Row: Robert Schrader, Megan Whalen, Ping He, Caleb Whittier, Ana Cartaya, Gyeong Bang.

2nd Row: R. Porter Ladley, Elizabeth Osborne, Alexandra Gittens, Edgar Alaniz, Shenell Collins, Kathryn Proe.

3rd Row: Austin Bartl, Scott Kirshner, Jessica Freeze, Amanda Carr, Murray Wan, Julian Smith-Jones, Kevin Denny.

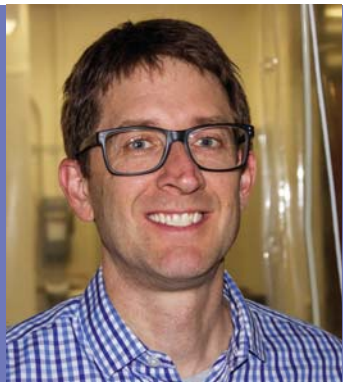
4th Row: Austin Bailey, Rachel Bonn, Joshua McGough, Norman Zhao, Paige Pizsel, Janson Ho.

5th Row: Michael Moskowitz, Douglas Bowlby, James Gayvert, Christopher Melnychuk.

# David W. McCamant

Associate Professor of Chemistry

Ph.D. 2004, University of California, Berkeley



## RESEARCH INTERESTS

Ultrafast vibrational spectroscopy of structural dynamics in photochemistry; vibrational coupling and relaxation; structural rearrangements and relaxation mechanisms in photo-excited nucleic acids; Ultrafast energy and electron transfer processes relevant for solar energy systems.

## CONTACT

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The **McCAMANT** group has had an exciting year with a good collection of publications and graduations. In August 2014, **KRISTINA WILSON (Ph.D. '15)** defended her thesis, "An Attempt at Direct Observation of Anharmonic Vibrational Coupling Constants with Two-Dimensional Femtosecond Stimulated Raman Spectroscopy." Kristina is now working at UCLA with their large freshman chemistry program. In November, **BARBARA DUNLAP (Ph.D. '15)** defended her follow-up to Kristina's work, "New Methods in Two-Dimensional Femtosecond Stimulated Raman." Barbara has taken a postdoc position at Ohio State University running their ultrafast laser facility. In April, **RANDY SABATINI (Ph.D. '15)**, who has spearheaded the growing Eisenberg/McCamant collaboration on solar hydrogen production, defended his Ph.D. work entitled "Excited State Dynamics, Molecular Interactions, and Electron Transfer in Systems for the Photochemical Production of Hydrogen." Randy has moved on to a postdoc position in Toronto working for Ted Sargent on new light-driven applications for semiconducting nanoparticles. Luckily, making up for all these graduations is the fact that **ZAK PIONTKOWSKI** joined the group in December. Zak is a UR Chemical Engineering major and has already made great strides in new Raman applications in the lab. Also heading to Canada was postdoc **COLLINS NGANOU**, who left in May for Cape Breton University to work with Martin Mkandawire. Collins finished up his outstanding work on DNA oligomer simulations and photochemistry this spring. This May we saw our stalwart undergraduates, **DANA BARNETT (B.S. '15)** and **CLAYTON STUMPF (B.S. '15)**, graduate with the many accolades that they certainly deserved. In the summer of 2015, we were happy to host two new Rochester undergrads, **GE SONG** and **AMANDA CARR**, and were sorry to say goodbye to **DAN MARK**, who has taken a job at Nike Golf.

**MIKE MARK** is building an excellent repertoire in the lab studying all of the photophysics behind successful light-harvesting for solar hydrogen production. He passed his qualifying exam in July with flying colors. **JOOHYUN LEE** is finalizing an outstanding paper on the ultrafast photophysics of dGMP and was able to attend the Time-Resolved Vibrational Spectroscopy (TRVS) Conference in Madison, Wisconsin this summer. That excellent meeting was run by another Rochester alum, **PROFESSOR MARTY ZANNI (B.S. '94)**. Dave was also able to attend TRVS and was surprised and honored to receive the TRVS Early Career award for "his contributions to femtosecond stimulated Raman spectroscopy of ultrafast photochemical reactions."



The McCamant group (left to right) : Ge Song, Dan Mark, Zak Piontkowski, Amanda Carr, Mike Mark, Joohyun Lee, Dave McCamant



Dave receives the TRVS Early Career Award from Marty Zanni (left, UR Chemistry B.S., 1994), Bucky the Badger and Ted Heilweil (right, NIST), June 25, 2015.

## John S. Muentner

Professor Emeritus of Chemistry

Ph.D. 1965, Stanford University



### RESEARCH INTERESTS

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

### CONTACT

[muentner@chem.rochester.edu](mailto:muentner@chem.rochester.edu)

For **JOHN MUENTER**, the past year has progressed much like the past few years; busy with nonacademic interests: travel, family, classical music, etc. The major family news is that his daughter received tenure as an experimental physical chemistry professor at Denison University in Granville, Ohio. John is a proud father who delights in his two grandchildren, ages 5 and 2. Molecular spectroscopy is still important to him and he continues to spend one week every couple of months working at MIT with Bob Field's graduate students. This year's International Molecular Spectroscopy Symposium included a mini-symposium on molecular spectroscopy in the classroom and John presented a paper on Chemistry 232, the p-chem lecture and lab course he developed with Bob Kreilick. No new papers this year, but the old ones are still being cited. According to the ISI database, John's papers have been cited more than 5900 times (yes, my ego is showing).

# Michael Neidig

Assistant Professor of Chemistry

Ph.D. 2007, Stanford University



## RESEARCH INTERESTS

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

## CONTACT

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**MICHAEL NEIDIG'S** group has continued to expand their research into non-precious metal catalysis in organic synthesis during their fourth year at Rochester. The group currently consists of six Ph.D. students, with **THERESA IANNUZZI** (U. Scranton) and **STEPHANIE CARPENTER** (U. Kentucky) joining the group this past fall. We also added the first postdoc to our group, **DR. SALVADOR MUÑOZ**, who joined us this past June after obtaining his Ph.D. from New Mexico State University working with Prof. Jeremy Smith. We were excited to have **JOE BAILEY (B.S. '15)** and **ARI SHAPS (B.S. '15)** with us again this past year, with both graduating this past May. We also had two new Rochester undergrads, **MEGAN WHALEN ('17)** and **FULEI PENG ('16)**, in the group who will continue with us next year. We were joined by numerous summer researchers in the group this year, including students from Monroe Community College, the University of Amsterdam and local high school students from the Rochester City School District. Our research on iron-catalyzed reaction in organic synthesis continues to expand, as evidenced by our publications this year on iron-NHCs, iron-bisphosphines and simple iron salt systems. We have also continued to work on a variety of iron-pincer systems of broad interest in inorganic chemistry. We were excited to receive research grants from the National Institutes of Health and the National Science Foundation this past year for our work in iron chemistry. Graduate students in the group were honored with some prestigious awards this past year, including **TESSA WOODRUFF** who received an NSF Graduate Fellowship and **STEPHANIE DAIFUKU** who received a Messersmith Dissertation Fellowship from the University of Rochester. Mike was also awarded an Alfred P. Sloan Research Fellowship. Stephanie presented her research at the Gordon Organometallics meeting in July and was selected for an oral presentation—a huge honor! Lastly, Mike has been busy traveling the world to spread the word about the group's projects, including trips to China in April and the EuCOMC meeting in Bratislava in July. As our research progresses this upcoming year, we look forward to completing several further studies and to continuing our foray into iron catalysis in organic synthesis.



*The Neidig Group (left to right): Jared Kneebone, Joe Bailey, Tessa Woodruff, Mike Neidig, Valerie Fleischauer, Theresa Ianuzzi, Stephanie Daifuku, Ari Shaps.*



# Bradley L. Nilsson

Associate Professor of Chemistry

Ph.D. 2003, University of Wisconsin, Madison



## RESEARCH INTERESTS

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

## CONTACT

nilsson@chem.rochester.edu

The **NILSSON** group continued to evolve during 2014-2015. **WATHSALA LIYANAGE** completed her Ph.D. studies and defended her thesis, "Functional and Structural Insight into Supramolecular Phenylalanine-Derived Materials", in April 2015. She has had several of her chapters accepted for publication to date. These include a description of multicomponent, coassembled hydrogels that act as fibronectin-mimetic materials for tissue culture applications. In addition, she published a seminal paper describing the evolution of self-assembled hydrogels into crystalline microtubes, enabling crystallographic studies that provide critical insight into the relationship between hydrogelation and crystallization of this class of materials as well as the packing architecture of the assembled materials. She made tremendous progress understanding and applying hydrogels derived from phenylalanine as materials during her Ph.D. studies. Additional manuscripts are currently under review and awaiting submission. Wathsala's work will influence research in the Nilsson group for years to come! She has joined Professor John Tovar's group (John's Hopkins University, Department of Chemistry) as a postdoctoral researcher and is working on organic photovoltaic molecules.

**JOHN DIMAIO** is also nearing completion of his Ph.D. studies. John started studies at the Law School at the University at Buffalo in the Fall of 2014. He has spent the last year commuting back to Rochester on the weekends to complete a few final experiments as well as writing his thesis and preparing manuscripts detailing his work with amyloid peptides as materials to prevent sexual transmission of HIV, among other applications. During summer 2015 he worked in the field of intellectual property at the University of Buffalo. He enjoys his studies and he's looking forward to defending and finishing up his Ph.D. thesis so that he can focus on only one job! John will be missed in the lab, not only for his research expertise, but also for the unique atmosphere he creates for his coworkers.

**ANNADA RAJBHANDARY** has also continued to make breakthroughs in the development of self-assembled materials derived from phenylalanine. She submitted a manuscript for a book chapter, "Self-Assembling Hydrogels" that will appear in the forthcoming "Fundamentals of Hydrogels" which will be published in late 2015. She is nearing completion of her Ph.D. studies and is beginning to write her thesis. She has begun the process of searching for post-graduate employment opportunities and we anticipate that she will defend her Ph.D. thesis either this Fall or early next Spring. She also got engaged to be married this year and we congratulate her on this exciting life development!

**DANIELLE RAYMOND** and **JEN URBAN** have kicked their research into high gear and are on the cusp of their first publications. They have had a productive year. Danielle has continued her study of rippled beta-sheet materials derived from the coassembly of enantiomeric peptides. Her work is opening up interesting new avenues for the application of these novel materials. Danielle was engaged this year to her fiancé, Clint. Congratulations to both of them! Jen, a member of both the Nilsson and Krauss groups, is working in an entirely new area: the application of quantum dots for super high resolution imaging of cellular processes. The work has been challenging, but highly interdisciplinary and interesting. Danielle and Jen have spent time at the Synchrotron (CHESS) at nearby Cornell University and have initiated collaborations with solid-state NMR spectroscopists to gain new structural insight into our self-assembled peptide materials. These new avenues of research will enhance our understanding of these interesting materials and enable the design of next-generation iterations.

**JADE WELCH** completed the departmental qualifying exams and has been advanced to candidacy for the Ph.D. degree. We congratulate her on this important achievement! She has had a strong start to her Ph.D. work and is moving ahead with research focused on the development of in vivo delivery agents for therapeutic oligonucleotides. We're excited by the direction of her work and look forward to an important year of progress for her.

**PAUL RUBEO** joined the Nilsson group as a new graduate student during the Fall 2014 semester. Paul completed his undergraduate studies at Nazareth College in education and subsequently entered the workforce as a high school teacher for several years. He decided to return to school to work towards a Ph.D. in chemistry. He has been an outstanding addition to the group and is focused on the identification of novel amyloid-binding molecules.

The Nilsson group has been fortunate to work with a number of talented undergraduate researchers in the last year. **BENJAMIN MEATH (B.S. '15)** and **RUIJIA ZHU (B.S. '15)** conducted senior research projects in the Nilsson lab last year, and have both successfully completed their undergraduate studies. Ben begins medical studies this fall and Ruijia accepted a research appointment at Harvard University beginning summer 2015. **SAGAR PATEL** and **JANSON HO** also conducted research in the Nilsson group during the last year. Sagar focused on self-assembly of the HIV-related SEVI amyloid and Janson opened up a new area of research in rippled beta-sheet formation in novel classes of peptides. Both students will continue their research projects in the coming year. This summer, Janson, along with **ADRIAN ROSENBERG, PAIGE PALMIERI,** and **ANA CARTAYA** (Monroe Community College), conducted summer REU research in the Nilsson group. They proved to be talented research students and Adrian and Paige will also continue their projects in the coming academic year. We're excited to have them in the lab for another year. In addition to these students, we welcome **KELSEY TUTTLE**, who joined the Nilsson group for the Fall 2015 semester. She will also carry out independent research in the Nilsson group during her senior year.

In addition to managing the Nilsson group, Brad has stayed busy this year as chair of the Harrison Howe Award Committee (Rochester Section of the American Chemical Society), Chair of the Department of Chemistry Graduate Studies Committee, and as the Chair of the Travel Grant Committee for the 24th American Peptide Symposium held summer 2015 and sponsored by the American Peptide Society. He completed his term of service (2013–2015) as an elected member of the Nominating Committee of the American Peptide Society this year as well. Brad taught the CHM 204 organic chemistry lecture for the third time (whew!) in Spring 2015 and also taught the Bioorganic Chemistry and Chemical Biology Course that same semester. The Nilsson group looks forward to another exciting year of progress and exploration!



*The Nilsson Group (left to right): Annada Rajbhandary, Brad Nilsson, Danielle Raymond, Jade Welch, Jen Urban, Adrian Rosenberg, Paige Palmieri, Janson Ho, Kelsey Tuttle, Paul Rubeo.*

# Lewis J. Rothberg

Professor of Chemistry

Ph.D. 1983, Harvard University



## RESEARCH INTERESTS

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

## CONTACT

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**LEWIS ROTHBERG'S** group focus remains the fundamental photophysics of luminescent conjugated polymer films and its implications for device applications of those materials. **BEN MARTIN** (soon to be married!) has great results on fluorescence from single polymer chains that explain many anomalous literature results and have stimulated new directions. Also, **RAJ CHAKRABORTY** has good results that help to understand the mysterious low field magnetic effects in organic light-emitting diodes (OLEDs). **CHRIS FAVARO'S** novel approaches to fabricating silver particle scattering layers and integrating them with OLEDs appears to be successful and we have done initial trials on devices made in Prof. Tang's labs and at a local manufacturer (OLEDWorks) interested in organic lighting. Each of the students is on a good trajectory to finish this year. **CHI-SHENG CHANG** has graduated with an exceptional thesis studying plasmonic effects on organic solar cells and taken employment in the semiconductor industry. In addition, **MILLARD WYMAN** has nearly completed his thesis in absentia and will likely receive his Ph.D. in the fall for what has turned out to be excellent work on delayed luminescence in conjugated ladder polymers. Chemical engineering MS student **CHEN ZHANG** has done fine spectroscopic work with senior scientists **AL MARCHETTI** and **RALPH YOUNG** to understand interfacial charging in model OLED structures. Obtaining research funding continues to be difficult and Lewis is spending more time in the lab with the graduate students and excellent undergraduates **MATT CARBONE** (photothermal absorption of ultrathin polymer films) and **CHRIS MELNYCHUK** (plasmon stabilization of fluorophores). Chris is now helping Lewis to transition some of his research to do transient vibrational spectroscopy aligned with a broad, exciting collaborative initiative in the department to work on sunlight driven catalysis to make transportation fuels from abundant materials. Lewis hopes to contribute to this exciting and important new direction, having realized that solving our energy problems in an environmentally responsible way is among the most important challenges facing modern society.

Both Lewis and the students presented work at a variety of ACS and Materials Research Society meetings. Most memorable for Lewis was giving the plenary talk at the 11th meeting on Optical Probes of Conjugated Polymers in Hong Kong. Lewis has attended every one of the 11 meetings (since 1992) and is co-founder of the very successful series with Valy Vardeny at the University of Utah. It still remains a flagship meeting for spectroscopy of organics, a field that remains problem and technology rich even nearly 30 years after **CHING TANG'S** seminal OLED work. Lewis has been blessed to see much of the science and technology evolve. The meeting was coupled with a memorable highlight of the year, sharing local sites and culture with friend and colleague Ching Tang, who is now on the faculty at a new institute at HKUST and a native of Hong Kong.

Lewis taught the junior level statistical thermodynamics (CHM 252), a course that continues to fascinate. He continues to teach the advanced spectroscopy lab (CHM 232) with a lot of help from **RAY TENG (B.S. '83, M.S. '87, M.B.A. '01)** and a strong cadre of teaching assistants. Lewis plans to work with colleagues in Physical Chemistry to add more modern labs to the course and update the manuals over the next several years. In the Fall, Lewis is excited to be teaching junior level quantum chemistry for the first time and looking forward to the rich understanding that preparing a course often brings.

Lewis remains director of the Materials Science program at the University, a Ph.D. and M.S. granting program that has now grown to nearly 50 students. The program is ably administered by **GINA EAGAN**. The faculty banded together for internal brainstorming meetings with the intent of preparing a strong Materials Research Center proposal to the NSF. We are also introducing new pedagogical and team-building programs for the cadre of materials science students.

Diffinity Genomics, a small biotechnology company formed to commercialize technology developed in our lab by **DR. HUIXIANG LI**, struggled once again this year but has nevertheless continued to sell products. Fortunately, the company's technology has attracted a buyer and has been purchased by Chiral Technologies, a much larger company capable of expanding sales and distribution. In part, this was possible because the patent on the UR-owned molecular separations technology at Diffinity's core was issued this past spring. It is likely that Lewis will continue to consult with Chiral Technologies on R&D to underpin future products in the genomics space that exploit some of the ideas developed by Diffinity. Lewis enjoyed recounting his entrepreneurial experience at a local ACS meeting and for the students in the NSF-REU summer program, and remains grateful to the department and University for the flexibility enabling him to learn and grow in different ways.

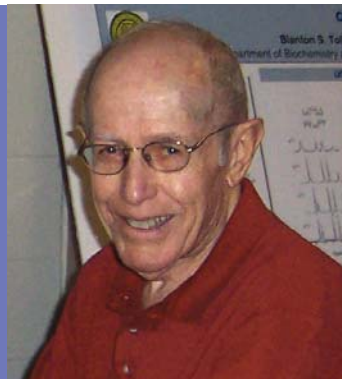
On a more personal note, Lewis lost his beloved mother Esther Conwell last fall, also a departmental stalwart whose affiliation with UR Chemistry long predates Lewis' employment. The department kindly sponsored a moving memorial service in March at the UR Chapel. Esther was widely cherished in the scientific community and garnered many awards. She continued to do publishable research until she died at 92 with manuscripts under review and more in preparation. She will be deeply missed at son Charles' Bar Mitzvah this year, Vivian's graduation from elementary school and other joyous family occasions.



## William H. Saunders

Professor Emeritus of Chemistry

Ph.D. 1952, Northwestern University



### RESEARCH INTERESTS

Ab Initio and Valence Bond Calculations of Proton Transfer and Elimination Reactions

### CONTACT

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The first activity of Summer 2014 was a visit to Claude and Gulchin in July. The highlight of the visit was a concert by Gulchin (piano) and a visiting friend (violin) in combination with a wine tasting. The summer also included a trip to the Stratford Shakespeare Festival and a visit by Anne and the girls to Rochester. In September, Zoe started college at Concordia University in Montreal. In November I attended the Physical Organic Minisymposium in Hamilton, Ontario. The band of oldtimers is diminishing but still there. The whole family spent Christmas in Rochester, the Christmas dinner postponed a day by an airline malfunction affecting Claude and Gulchin. The big trip of the year was a tour of Portugal sponsored by the local PBS station, WXXI. We stayed in a variety of Pousadas, a chain of hotels in repurposed historic buildings. Our last stop was an ultramodern hotel inside a 15th century fortress. We had plenty of good wine and a dinner in a Fado restaurant (Fado refers to a usually mournful style of singing popular in the country). The computational study of orientation in elimination reactions that Scott Gronert and I had been working on finally was written up and submitted to the *Journal of Organic Chemistry*.

## Wolf-Udo Schröder

Professor of Chemistry

Ph.D. 1971, University of Darmstadt, Germany



### RESEARCH INTERESTS

Basic and applied nuclear science: dynamics of complex nuclear reactions at intermediate and high energies; dissipation, relaxation and other transport phenomena; non-equilibrium effects; thermodynamics of nuclear disintegration and transmutation; the equation of state of nuclear matter. Beyond the mean field: correlations and clusterization of nuclear matter. Light-ion reactions in a thermonuclear environment. Chemi- and physisorption of tritium in metals.

### CONTACT

schroeder@chem.rochester.edu

**W. UDO SCHRÖDER'S** Nuclear Science Research Group has continued research in radiochemistry, heavy-ion reaction dynamics, advanced detector development, as well as development of Laser Ion Acceleration for Nuclear Science (LIANS).

Work by two Ph.D. students (**ERIC HENRY** and **SHETH NYIBULE**) continued on results obtained in heavy-ion experiments conducted at the Italian laboratory LNS Catania at low and intermediate bombarding energies. Technical evaluations of a new type of plastic scintillator material were published and received unusually strong interest in the community. More than 528 downloads of the paper occurred within the period of a few months after publication.

Radiochemical investigations of transport phenomena for tritium in metals and of tritium adsorption on metallic surfaces have been continued. A combination of thermal desorption and plasma induced sputtering measurements on a series of different materials has produced comprehensive sets of data allowing one to critically evaluate industrial

methods of tritium recovery. Further progress has been made explaining the mechanism of diffusion through, and desorption from, tritiated metals.

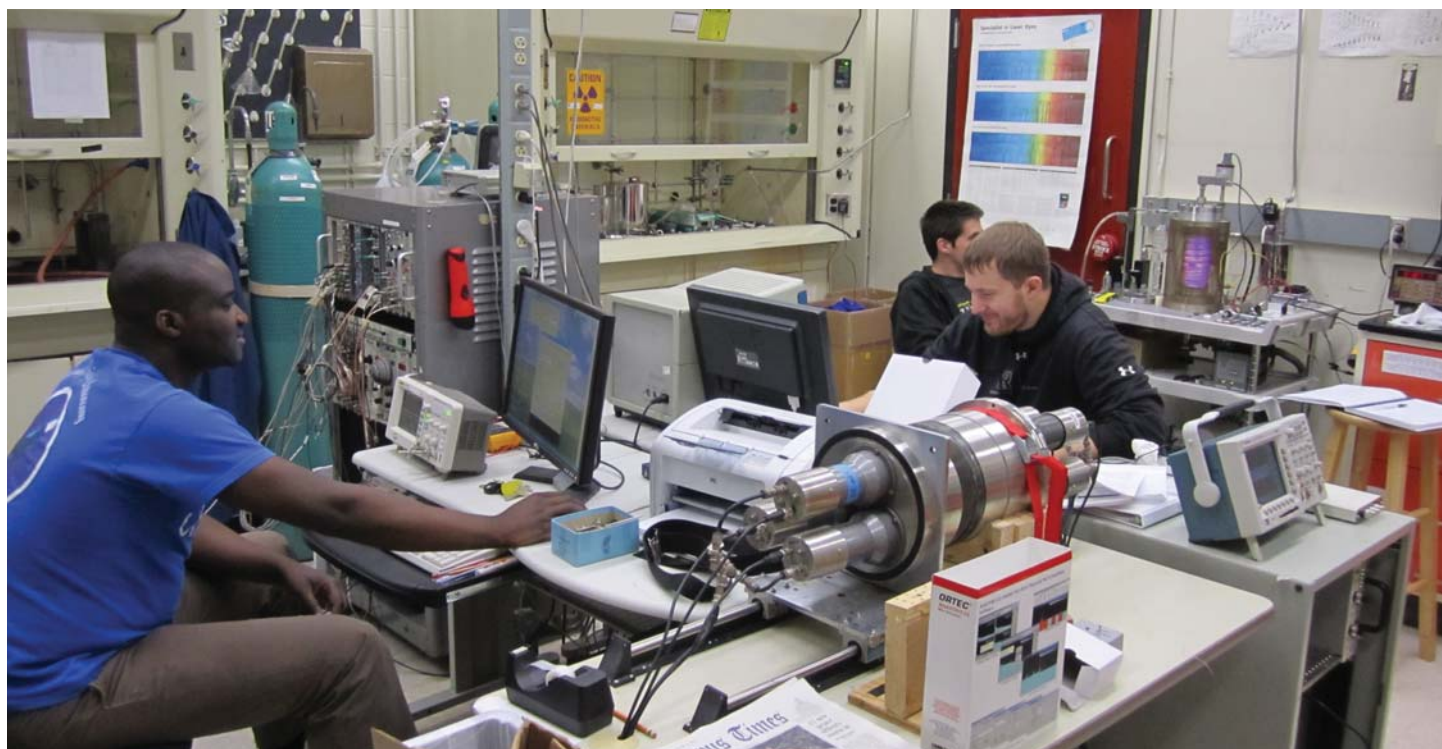
Further experiments on the LIANS (Laser Ion Acceleration for Nuclear Science) project at the Omega/EP laser system have been successful in producing well-controlled beams of MeV deuterons. Several laser shots have been used by the group to measure neutrons emitted in the reaction  ${}^9\text{Be}(d, n){}^{10}\text{B}$ . Some lessons were learned for designing the next set of improved  ${}^9\text{Be}$  target.

Several group members attended international conferences and presented results of their research. **MATT SHARPE** gave a presentation about his Ph.D. tritium transport work at a topical conference on energy technologies and materials in Austin, Texas. Eric Henry presented results of his Ph.D. work in an invited talk entitled “Evidence for a Novel Prompt Fusion-Fission Mode” at the 2015 Gordon Research Conference on Nuclear Chemistry in New London, New Hampshire in May/June 2015. Sheth Nyibule gave a poster presentation on his thesis work at the same conference.

Udo gave a week of lectures at the 2014 ACS Nuclear Chemistry Summer School at Brookhaven National Laboratory and presented a talk on the University of Rochester Nuclear Science program at a workshop preparing for the next NCAC Long Range program. The Division of Nuclear Chemistry and Technology of the American Chemical Society sponsors and administers the summer schools in nuclear and radiochemistry which are funded by the U.S. Department of Energy. Students participating in the six week summer program at Brookhaven National Laboratory have the opportunity to visit research sites, attend guest lecture series, and meet and interact with prominent research scientists working in nuclear and radiochemistry.



*Udo lecturing at the 2014 ACS Nuclear Chemistry School at Brookhaven National Laboratory*



# 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 influenza RNA.

## CONTACT

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The **TURNER** group is combining interests in RNA structures in influenza A and methods for predicting 3D structures from sequence. Two secondary structures predicted in 2011 by **WALTER MOSS (Ph.D. '11)** and **SAL PRIORE (Ph.D. '13)** were confirmed by chemical mapping. One is a multi-branch loop mapped by **TIAN JIANG (M.S.'11)** and the other a pseudoknot mapped by **ANDY KAUFFMAN** and **SAL PRIORE**. **JON CHEN (Ph.D. '15)** collaborated with **SCOTT KENNEDY** to determine by NMR the 3D structure of a hairpin containing a 3' splice site that allows generation of the mRNA for an essential protein, called M2. We are unaware of other structures known for 3' splice sites and Jon's structure defines a potential therapeutic target. All these structures were published in *Biochemistry*.

The group continues to collaborate with **LUIS MARTINEZ-SOBRIDO** in the Microbiology Department to test for functions for the influenza structures and for compounds to inhibit function. Tian and long time collaborators, **ELA** and **RYSZARD KIERZEK** from the Institute of Bioorganic Chemistry in Poznan, Poland, have taken up these quests. **ELA LENARTOWICZ**, the first Ph.D. student from Ela Kierzek's lab, started a postdoc in the Turner lab to also join the quests. Oligonucleotides are promising inhibitors of RNA function and Ryszard, Ela and Doug wrote a review of their microarray method for identifying potential sites to target with oligos. Completion of this review was facilitated by a week spent by Doug at the Institute in Poznan.

Doug, Scott, and Ryszard were coauthors of a paper from the Das lab at Stanford reporting a new approach to determine NMR structures of RNA on the basis of chemical shifts. In Jon Chen's paper, results from that method were compared with those from a standard NOE distance method and the comparisons revealed dynamics of influenza loops. Tian is collaborating with Luis Martinez-Sobrido to test how site directed mutations in predicted secondary structures affect virus propagation. Luis, Doug, and **STEPHEN DEWHURST** in Microbiology received a University Research Award to support part of their collaboration.

The ultimate goal is to predict RNA structure on the basis of sequence and physics. Toward this end, **DAVE CONDON (Ph.D. '15)** spearheaded collaboration with Scott, Brendan Mort (UR Center for Integrated Research Computing), Ryszard, and **ILYAS YILDIRIM (PHYSICS Ph.D. '08)** to compare NMR spectra of single stranded, unpaired tetramers, AAAA, UUUU, CAAU, and GACC, with predictions from extended molecular dynamics (MD) simulations (36  $\mu$ s for each tetramer). The simulations use classical physics to approximate the quantum mechanics of RNA. The results reveal that there are a lot of challenges remaining to approximate molecular interactions well enough to predict RNA 3D structure from sequence. Moreover, unpaired tetramers are excellent systems for benchmarking progress.

Dave Condon took a postdoctoral position in bioinformatics at the Medical Center of the University of Pennsylvania. Sal Priore received his M.D. and also moved to the Medical Center at Penn. Jon Chen started a postdoc with **MATT DISNEY (Ph.D. '02)** at Scripps in Florida. Tian Jiang will graduate in Fall 2015 and has accepted a research position at Abbott Labs in Dallas. She will join a group with Turner alums, **JIM HART (Ph.D. '08, M.D. '10)** and **TIANBING XIA (Ph.D. '99)**. Two other Turner alums are also in Dallas, **DIANE BATES (Ph.D. '81)** now retired from Abbott Labs, and **JAMES KIM (Ph.D./M.D. '97)** an Assistant Professor at the University of Texas Southwestern Medical Center. It's a small world.

A new graduate student, **JIANBO ZHAO**, joined the group to collaborate with **DAVE MATHEWS (Ph.D. '01, M.D. '03)** and **SCOTT KENNEDY** to improve our understanding of molecular interactions that determine RNA structure. Graduate students **KYLE BERGER** and **ANDY KAUFFMANN** are contributing to the effort by determining NMR structures to benchmark predictions.

In news from alumni, **WALTER MOSS** received an NIH K99 Pathway to Independence Award that will fund his postdoc in Joan Steitz's lab at Yale and also help support start up when he accepts a faculty position. **BLANTON TOLBERT (BIOPHYSICS Ph.D. '07)** was promoted to Associate Professor with tenure in the Chemistry Department at Case Western Reserve University.

Doug enjoyed spending time with **PHIL BEVILACQUA (Ph.D. '93)** at Penn State and at the RNA Dynamics meeting in Telluride. Doug also presented the group's results at UR's "Second Friday Science Social," the annual symposium, "From Genome to Function," of the Italian Biophysics and Molecular Biology Society, and at the Albany College of Pharmacy and Health Sciences (ACPHS). The latter talk was part of a symposium celebrating the inauguration of **GREG DEWEY (Ph.D. '79)** as President of ACPHS. The next day, Doug had the pleasure of helping introduce Greg to the ACPHS community, informing them that he grew up as a Pittsburgh Pirate fan, and warning them that he had in his office a baseball bat from Bill Mazerowski so that they should only disagree with Greg in an agreeable way.

After a Fall sabbatical, Doug taught the Spring afternoon section of General Chemistry, along with part of the Biophysical Chemistry course, and a "critical thinking" course in the School of Medicine and Dentistry. After spending much of the last 40 years teaching General Chemistry, Doug decided that he has learned most of the concepts, so he resigned from teaching in order to spend more time applying the concepts to RNA research.

## Daniel J. Weix

Associate Professor of Chemistry

Ph.D. 2005, University of California, Berkeley



### RESEARCH INTERESTS

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

### CONTACT

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Research in **PROFESSOR WEIX'S** group is focused on the development of new catalytic methods for forming C-C and C-X bonds, with a particular emphasis on understanding mechanism and the use of first-row transition metals. The major focus of the group continues to be the selective cross-coupling of two electrophiles and the use of earth-abundant, first-row metals. Advances this year include the development of co-catalysts that, along with nickel, allow the enantioselective opening of meso-epoxides (titanium), the coupling of benzyl mesylates with aryl halides (cobalt), and a remarkable cross-Ullman reaction between aryl bromides and aryl triflates (palladium). Cross-electrophile coupling continues to grow in importance, both in academia (several groups have begun working in the area this year) and in industry (Novartis, Boehringer-Ingelheim, Pfizer, Merck). We are grateful for new industrial funding from Boehringer-Ingelheim, Novartis, and Pfizer! Although 2015 is already our most productive year ever (9 publications), many more exciting results are nearing completion!





*The Weix group: (left to right) Front row: Shenell Collins, Norman Zhao; Back row: Alex Wotal, Laura Ackerman, Kierra Huihui, Stephanie Rugg, Yang Zhao, Jill Caputo, Keywan Johnson, Astrid Olivares, Don Batesky, Zulema Melchor, Dan Weix*

Daniel continued teaching freshman this year, but switched to the Freshman Organic Chemistry lecture. His first year was a great success, in no small part because of the wonderful students and the enthusiastic workshop leaders. In addition to lecturing the students, Daniel was able to bring demonstrations back into the classroom, starting with the nylon-6,6 demo and a 2-L-scale luminol demonstration. He plans to expand into more demonstrations next year. Chemistry 210 gave Daniel the opportunity to continue to use the fantastic 102 teaching lab space and to work with the future chemistry majors. Finally, a second paper based upon 234 Lab work was published with undergraduate authors based upon a new experiment developed by **STEPHANIE RUGG (Ph.D. '15)** and Daniel.

The group was fortunate to be recognized with a variety of awards and honors this past year. Recent alumni **RYAN RIBSON (B.S. '14)** was a runner-up for the NSF Graduate Research Fellowship and graduate student **KEYWAN JOHNSON** was chosen as an awardee! Keywan was also awarded the HHMI Gilliam Fellowship this spring along with the Sherman Clarke Fellowship last fall in recognition of his accomplishments in labwork, classwork, and teaching performance. **KEITH HILFERDING (M.S. '14)** and **KIERRA HUIHUI** both received the W. D. Walters Teaching Award last fall for their teaching performance in CHM 234 Lab. **LUKIANA ANKA-LUFFORD** and Stephanie were both awarded the Weissberger Memorial Fellowship in recognition of their research accomplishments. In addition, Lukiana was awarded the Division of Organic Chemistry Travel award this past winter and **JILL CAPUTO** was selected to attend the 2015 Division of Organic Chemistry Graduate Research Symposium in Austin, TX. **ALEXANDER WOTAL** returned from his one year co-op with the Glaxo-SmithKline Anti-Bacterial team in May. Daniel Weix was invited to speak at Organic Reactions and Processes Gordon Research Conference and organized a symposium on "Base Metal Catalysis" at the ACS Green Chemistry and Engineering Conference in 2015. Our research program was recognized this year with the Novartis Early Career award (one of two chosen internationally this year; Ryan Shenvi of Scripps was the other 2014 awardee), and a second Green Chemistry Award from the Pfizer Groton Green Chemistry Team.

This year we had four departures and welcomed four new researchers. **DR. NICK GOWER** completed his Pfizer-funded postdoc in June and returned to sunny England for a Postgraduate Certificate of Education (PGCE) on the School Centred Initial Teacher Training (SCITT), which is sponsored by the Royal Society of Chemistry. Stephanie successfully defended her thesis in August and will be a visiting assistant professor at SUNY Oswego this coming academic year. Keith Hilferding completed his Master's degree and took a job with the aptly-named Chemicals Incorporated in Texas. Finally, **ADAM HAAS (B.S. '15)**, who was mentored by **YANG ZHAO** graduated and moved to the actually-sunny Colorado State University for graduate school.

New additions include first-year graduate students **ZULEMA MELCHOR** and **ASTRID OLIVARES**. Zulema graduated from University of Texas at Brownsville and was an NSF REU student in 2013, working with **LAURA ACKERMAN**. Astrid obtained her Bachelor's degree from California Lutheran University, where she worked on C-H activation with John Tanaci. We welcomed undergraduates **ANDREW OLSEN** and **NORMAN ZHAO** into the group, who are mentored by Stephanie and Jill. Andrew Olsen was an NSF REU student in the summer of 2014. This summer, we had the pleasure of hosting both Norman and **SHENELL COLLINS** for the NSF REU. Shenell is from St. John's University, and she worked with Yang this summer. **DONALD BATESKY** is still going strong as a research associate in the lab with macroscale synthesis, where he specializes in heterocycles, in order to supplement the graduate student's work! His playful demeanor and vast knowledge is always a pleasure to have in the lab.

Kierra and Keywan both passed their oral exams and have advanced to candidacy. Kierra also presented her third-year talk entitled "Gold-Catalyzed Transformations of Alkynyl Aryl Sulfoxides." Zulema Melchor and Astrid Olivares were class-leaders for a group of middle school students in the Horizons summer program at the University of Rochester this summer, a program started by Laura Ackerman a few years ago. Several group members participated in conferences and symposiums across the country. Daniel, Nick, Laura, Stephanie, and Yang all attended the ACS National Meeting in San Francisco, CA in August of 2014. Lukiana attended the ACS National Meeting in Denver, CO in April 2015, and Jill and Keywan participated in the ACS National Meeting in Boston, MA in August 2015.

For the Weix group, it was the year of weddings! The Weix-Wu family traveled to Wisconsin for the wedding of Daniel's brother, Stephen, to Lindsey Paulsen. It was a wonderful day and a rare chance to see some of the very large Weix extended family. In June, Stephanie and Kyle Rugg were married at Peek n' Peak ski resort in Pennsylvania where several Weix and Boeckman group members were in attendance. A little more than a month later Lukiana married Wonder Amedzo on a beautiful August day in Pomona, NY with several chemistry department members at the celebration. In other exciting news, **DANIEL EVERSON (Ph.D. '13)**, his wife Kelsey, and daughter Cora welcomed their second daughter, Autumn, in May. Daniel Weix's children, Elliott (10), Madeleine (8), and Amalia (6), continue to keep him and his wife, Stella, busy. Elliott has taken up string bass and piano, Madeleine continues to enjoy gymnastics, and Amalia enjoys doing a little bit of everything.

In group alumni news, Ryan Ribson completed his first year at Caltech and joined the group of Jonas Peters. **MICHAEL ROBO (B.S. '14)** also completed his first year at the University of Michigan and has started working with John Montgomery. **MATTHEW LOVELL (B.A. '14)** has spent the past year working as a firefighter and EMT and has been volunteering at Akron Children's Hospital in the ER. Matthew is furthering his education at Case Western Reserve University where he will be earning a Master's in Medical Physiology. **MICHAEL PRINSELL (Ph.D. '13)** finished up his teaching postdoctoral position with Nancy Mills at Trinity University and accepted a tenure-track assistant professor position at Monmouth College where he will begin teaching in the fall of 2015. **DANIEL EVERSON** is currently a visiting assistant professor at St. Olaf College and is applying for permanent positions this fall. **RUJA SHRESTHA (Ph.D. '13)** finished her postdoc with John Hartwig and started working for Rennovia, a company dedicated to the development of new catalysts for the conversion of renewable feed stocks into specialty chemicals. **DR. SOUMIK BISWAS** finished up his postdoctoral position with John Gladysz at Texas A&M University and began a new postdoc with Boehringer Ingelheim in Ridgefield, CT. Congratulations and best wishes to all!



*Daniel and members of the Weix group at the graduation of Adam Haas.*

## ROBERT K. BOECKMAN, JR.

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## KARA L. BREN

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Effects of Protein Structure on Iron-Polypeptide Vibrational Dynamic Coupling in Cytochrome c. M. G. I. Galitano; S. E. J. Bowman; J. G. Kleingardner; S. Martin; J. Y. Zhao; W. Sturhahn; E. E. Alp; K.L. Bren; S. J. Elliott, *Biochemistry*, **2015**, *54*, 1064.

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## JOSEPH P. DINNOCENZO

Accurate Oxidation Potentials of 40 Benzene and Biphenyl Derivatives with Heteroatom Substituents. P. Luo; A. M. Feinberg; G. Guirado; S. Farid; J. P. Dinnocenzo, *J. Org. Chem.*, **2014**, *79*, 9297.

Transition from Charge-Transfer to Largely Locally Excited Exciplexes, from Structureless to Vibrationally Structured Emissions. R. H. Young; A. M. Feinberg; J. P. Dinnocenzo; S. Farid, *Photochem. Photobiol.*, **2015**, *91*, 624.

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## RICHARD EISENBERG

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## SAMIR FARID

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## JAMES M. FARRAR

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Enzymatic C(sp<sup>3</sup>)-H Amination: P450-Catalyzed Conversion of Carbonazidates into Oxazolidinones. R. Singh; J. N. Kolev; P. A. Sutura; R. Fasan, *ACS Catal.*, **2015**, *5*, 1685.

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## **WILLIAM D. JONES**

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## JOHN S. MUENTER

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## DOUGLAS H. TURNER

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## DANIEL J. WEIX

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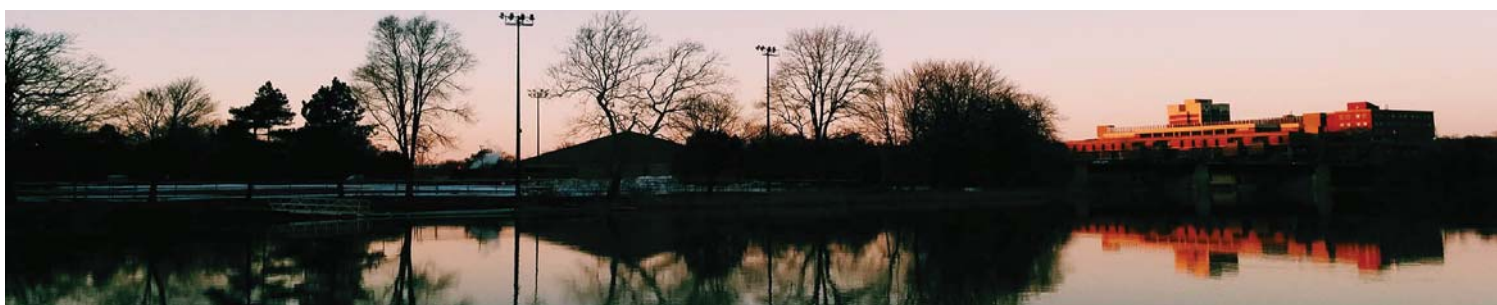
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# Commencement

## Bachelors and Masters Degrees Awarded in Chemistry

### 2015 BACHELOR OF SCIENCE

Dylan Abrams <sup>3†</sup>  
Joseph Bailey <sup>1</sup>  
Danielle (Dana)  
Barnett <sup>2†</sup>  
Hong-Ting (Natalie)  
Chan <sup>2</sup>  
John DeCoursey <sup>1</sup>  
Adam Haas <sup>1</sup>  
Chitavi Maulloo <sup>3†</sup>

Kevin McClelland <sup>3†</sup>  
Ari Shaps  
Taylor Sodano <sup>1\*\*</sup>  
Clayton Stumpf <sup>2</sup>  
Johnson Truong  
Lauren Weber <sup>3†</sup>  
Zhijie Wu <sup>3†</sup>  
Nan Yang

### 2015 BACHELOR OF ARTS

Alexandra Born <sup>2</sup>  
Jialu Chen  
Marion Dullea <sup>1</sup>  
Nathan Freeman <sup>1\*\*</sup>  
Nicholas Hill <sup>3†</sup>  
Blythe Hospelhorn <sup>1</sup>  
Chee Yung Kong <sup>\*</sup>  
Alexander Kozlov  
Qi Ying (Queenie) Li <sup>3†</sup>

Zi-Rou (JoJo) Liew <sup>3</sup>  
Jack Maguire <sup>1</sup>  
Rina Minato <sup>1\*\*</sup>  
Annah Moore  
Leti Nunez <sup>2†</sup>  
Shane O'Neil <sup>\*</sup>  
Daniel Salazar  
Juan Manuel Vasquez

<sup>1</sup>Distinction <sup>2</sup>High Distinction <sup>3</sup>Highest Distinction <sup>†</sup>Phi Beta Kappa  
<sup>\*</sup>Take 5 Scholar (beginning) <sup>\*\*</sup>Take 5 Scholar/KEY Program (finishing)



*Class of 2015 Bachelor's Degree Recipients*

### 2015 MASTER OF SCIENCE

Hanan Alwaseem  
Rachel Carey  
Saikat Chakraborty  
Valerie Fleischauer  
Abigail Freyer  
Patrick Harrington  
Emily Hillenbrand

Kierra Huihui  
Keywan Johnson  
Zhi Li  
Dan Mark  
Michael Mark  
John McAnany  
Andrew Owens

Kyle Rugg  
Heidi Schlager  
Brian Sheldon  
Matthew Sleck  
Eric Stoutenburg  
Alexander Stwertka  
Sreyoshi Sur

Oliver Swart  
Peter Thayer  
Lidong Wang  
Jade Welch  
Tessa Woodruff  
Jianbo Zhao

# Student Awards

## DEPARTMENT AWARDS

**Dr. E. W. and Maude V. Flagg Award**  
Dylan Abrams

**John McCreary Memorial Prize**  
Nicholas Hill

**ACS Rochester Section Award**  
Kevin McClelland

**ACS Inorganic Chemistry Award**  
Lauren Weber

**ACS Organic Chemistry Award**  
Zhijie Wu

**ACS Analytical Chemistry Award**  
Chitavi Devi Maulloo

**Chemistry Department Award**  
Danielle Barnett  
Qi Ying Li  
Zi-Rou Liew  
Clayton Stumpf  
Nan Yang

## COLLEGE AWARDS

**Janet Howell Clark Prize**  
Chitavi Maulloo

**Catherine Block Memorial Fund Prize**  
Rachel Kasimer  
Christine Ziegler

## TEACHING AWARDS

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

**Carl A. Whiteman, Jr. Teaching Award**  
Dylan Abrams  
Danielle Barnett  
Matthew Carbone  
Leti Nunez





## ENDOWED DEPARTMENT FELLOWSHIPS

### Robert & Marian Flaherty DeRight Fellowship

Malik Al-Afyouni  
Andrew Kauffmann

### Moses Passer Fellowship

Kyle Biegasiwicz  
Douglas Tusch

### Elon Huntington Hooker Fellowship

Laura Ackerman  
Stephanie Daifuku  
Banu Kandemir  
Joshua Kolev  
Yang Zhao



### Arnold Weissberger Fellowship

Lukiana Anka-Lufford  
Stephanie Dorn  
Adam Feinberg  
Jared Kneebone  
Gregory Pilgrim



### Samuel A. & Ellen F. Lattimore Fellowship

Rachel Carey  
Valerie Fleischauer  
Abigail Freyer  
Tessa Woodruff  
Jing Yuwen

### Robert L. & Mary L. Sproull Fellowship

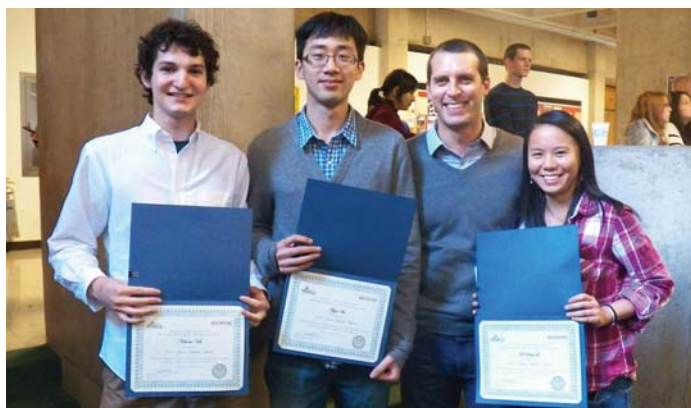
Jennifer Urban

## PHI BETA KAPPA

Dylan Abrams  
Danielle Barnett  
Nicholas Hill  
Qi Ying Li  
Chitavi Devi Maulloo  
Kevin McClelland  
Leti Nunez  
Lauren Weber  
Zhijie Wu



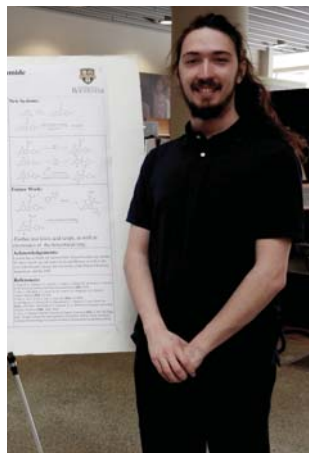
## Student Awards and Accolades



*Fasan Group members Nick Hill, Abe Wu and Queenie Li receiving their awards in Fall 2014.*

This year's John McCreary Memorial Prize winner, **NICHOLAS HILL (B.A. '15)**, has worked in the Fasan lab since spring of his freshman year developing new methods for synthesizing cyclic peptides. This prize was established in 1985 in tribute to the high academic and scientific standards and the personal dedication of John James McCreary who received his B.S. degree in Chemistry in 1975. Nicholas participated in both REU and study abroad programs in Sweden and Switzerland, and graduated with the Chemistry Department's highest distinction honors. He has started graduate studies in chemistry at the University of Colorado in Boulder.

**DYLAN ABRAMS (B.S. '15)** was selected to receive the Dr. E.W. and Maude James Award which recognizes outstanding performance and promise in chemistry. This award was established in 1982 as an endowed fund by Dr. John J. Flagg to recognize outstanding performance and promise in chemistry by a graduating senior. Dylan did undergraduate research with Alison Frontier and will be attending Princeton University to pursue a Ph.D. in Chemistry. After conducting her senior research in the Bren lab, **LAUREN WEBER (B.S. '15)** won the ACS



*Lauren Weber and Dylan Abrams at the 2015 Senior Poster Session.*

Inorganic Chemistry Award, and was pleased to be offered a position at Bausch & Lomb doing sample processing and research in their contact lens division.

**ZHIJIE (ABE) WU (B.S. '15)** will bring his ACS Organic Chemistry Award with him when he moves out to the midwest to join the Ph.D. program in Chemistry at the University of Wisconsin-Madison. **KEVIN McCLELLAND (B.S. '15)** was the recipient of the ACS Rochester Section Award, given to a senior with an outstanding academic record. He was recognized during the ACS Annual Rochester Section Undergraduate Research Symposium and his name is now displayed on a plaque in the department. He is in the doctoral program in chemistry at Northwestern University and will continue his research in the physical chemistry of quantum dots in the group of Professor Emily Weiss.



*Danielle Barnett, Leti Nunez, and Matt Carbone.*

This year's recipients of the Carl A. Whiteman, Jr. Teaching Award for exemplary teaching by an undergraduate were **DYLAN ABRAMS (B.S. '15)**, **DANIELLE BARNETT (B.S. '15)**, **MATTHEW CARBONE**, and **LETI NUNEZ (B.A. '15)**. Carl Whiteman graduated from the University of Rochester in 1950 (B.S. Physics) and worked continuously in the department until his retirement in 1986. His enthusiasm and dedication to laboratory teaching made him a legendary figure among undergraduate chemistry majors.



*Zi-Rou Liew, Clayton Stumpf, and Nan Yang.*

Chemistry Department awards went to **DANIELLE BARNETT (B.S. '15)**, **QIYING (QUEENIE) LI (B.A. '15)**, **ZI-ROU LIEW (B.A. '15)**, **CLAYTON STUMPF (B.S. '15)**, and **NAN YANG (B.S. '15)**. These awards are given to seniors in recognition of outstanding scholarship in the study of chemistry.

**CHITAVI DEVI MAULLOO (B.S. '15)** was honored to receive both the ACS Analytical Chemistry Award and the Janet Howell Clark Prize. Established by the University, this prize is given to the senior woman who has shown the greatest promise in creative work in one of the following fields - Physics, Chemistry, Biology, or Astronomy - and has shown outstanding versatility in the mastery



of the allied fields. Chitavi's interest in nanoparticles used for biological applications began in a summer internship before her junior year when she went to the EPFL in Switzerland, and then continued her research with Dr. Lisa DeLouise at the medical center. Chitavi graduated with

the highest distinction chemistry honors and was elected to Phi Beta Kappa. As a junior, Chitavi was also the recipient of the Catherine Block Memorial Fund Prize. Chitavi will be continuing her education as a Ph.D. student in Molecular Engineering at the University of Chicago.

This year there are two recipients of the Catherine Block Memorial Fund Prize, established in the memory of



Catherine Block, an exceptional UR Chemistry student: **RACHEL KASIMER**, and **CHRISTINE ZIEGLER**. This University award is given to women in the junior class in recognition of their outstanding ability and achievement in the field of science. Rachel is a member of the Frontier group, and Christine has been working in the Fasan lab.

Congratulations to **BRIAN SHELDON (M.S. '15)** who was selected to receive the Edward Peck Curtis Award for Excellence in Teaching by a Graduate Student which is given to an exceptional teaching assistant who is selected in a University-wide competition. The nomination is comprised of letters of support from the Chair, faculty, and students.



The department gave four W.D. Walters Teaching Awards this year to **REBECKAH JOHNSON BURKE**, **RACHEL CAREY**, **ABIGAIL FREYER**, **ANALUZ MARK**, and **KYLE RUGG**. This award, memorializing the late Professor Walters, recognizes outstanding undergraduate teaching by graduate teaching assistants and their commitment and achievements.



*W.D. Walters awardees: Analuz Mark, Abby Freyer, Rachel Carey, Rebeckah Johnson Burke, and Kyle Rugg.*

Two graduate students were recipients of the Robert and Marian Flaherty DeRight Fellowship, established in 1984 as a tribute to Dr. DeRight by his wife, Marian. Both received their Bachelor's degrees from the University in 1931, in chemistry and romance languages, respectively. Robert continued his chemistry studies at UR and received his Ph.D. in 1935 with advisor Professor Edwin Wüg in physical chemistry. Dr. DeRight was a lifelong valued member of the ACS, and both he and his wife were very active in UR alumni affairs. The fellowship

provides **MALIK AL-AFYOUNI** and **ANDREW KAUFFMANN** with graduate support for one year.

Five Chemistry graduate students were selected to receive 2014-15 Elon Huntington Hooker Fellowships, which are supported by a gift from the wife of Elon H. Hooker, a graduate and Trustee of the University, and founder of the Hooker Electrochemical Company. The recipients are **LAURA ACKERMAN, STEPHANIE DAIFUKU, BANU KANDEMIR, JOSHUA KOLEV,** and **YANG ZHAO.**

The purpose of the Arnold Weissberger Fellowship in Chemistry is to reward and encourage outstanding research achievement and the potential for continued growth. This year's deserving recipients are **LUKIANA ANKA-LUFFORD, STEPHANIE DORN, ADAM FEINBERG, JARED KNEEBONE,** and **GREGORY PILGRIM.** Each fellow receives additional financial support and the funds to travel to a major scientific meeting to report the results of his or her research.

**KYLE BIEGASIEWICZ** and **DOUGLAS TUSCH,** both graduate students in the Boeckman group, were selected to receive the 2014-15 Moses Passer Fellowship which was established in 2009 by Mrs. Dorothy Rosenberg-Passer in memory of her husband. Dr. Moses Passer received his B.S. degree in Chemistry from the University of Rochester in 1945 and his Ph.D. in Organic Chemistry from Cornell in 1948. After a distinguished career as a professor at the University of Minnesota in Duluth, Dr. Passer served as director of Education at the ACS for more than two decades.



*Doug and Kyle outside a fire drill.*

Five outstanding graduate students were recipients of the 2014-15 Samuel A. & Ellen F. Lattimore Fellowship which was established to honor Professor Lattimore who was associated with the University of Rochester for more than 40 years and was Chair of the Department of Chemistry from 1867 to 1908. The fellowship winners are **VALERIE FLEISCHAUER, RACHEL CAREY, ABIGAIL FREYER, TESSA WOODRUFF,** and **JING YUWAN.**



*Jennifer Urban with Todd Krauss*

**JENNIFER URBAN,** a joint member of both the Nilsson and Krauss groups, was nominated by the Chemistry faculty and selected by the University Dean of Graduate Studies for the third year in a row to receive the Robert L. and Mary L. Sproull Fellowship, the most prestigious fellowship awarded by the University of Rochester. Jennifer's research focuses on pairing semiconductor quantum dots, which possess size-tunable optical and electronic properties, with peptide hydrogels and studying their combined properties.

Congratulations to **KEYWAN JOHNSON** (Weix group) and **TESSA WOODRUFF** (Neidig group) for being recipients of National Science Foundation Graduate Research Fellowships. The fellowship provides up to three years of graduate study support for students pursuing doctoral or research-based master's degrees, and also offers international research and professional development opportunities for students. Recent UR Chemistry alumni also received honorable mentions for their fellowship applications: **KEVIN McCLELLAND (B.S. '15), RACHEL KELEMEN (B.S. '13), RYAN RIBSON (B.S. '14),** and **JAMES SHANAHAN (B.S. '14).**



*Adam Feinberg with Dr. Elliot Richman*

**ADAM FEINBERG**, a member of the Dinnocenzo group, was chosen to be the first recipient of the Elliot and Laura Richman Travel Award to support his attendance at the Physical Organic Chemistry Gordon Conference in June 2015. Adam met with Dr. Richman during Meliora Weekend to discuss his experience at the conference and thank him for the opportunity to share his research and interact with colleagues in his field.

**AMANDA PRESKE** received a poster award from LANL QD scientist Dr. Victor Klimov at the “20 years of QDs conference at Los Alamos” held in Santa Fe, New Mexico in April 2015. “This research, which started two decades ago with a handful of fragments of semiconductor-doped colored glasses, has evolved into a wide-ranging program spanning different areas of quantum dot science from synthesis and spectroscopy to theory and devices,” said Victor Klimov, the NanoTech team’s

leader and the founder of the Laboratory’s quantum dot program. Klimov gave a special introductory address at the conference with his personal perspective on the field’s evolution.

**ZHENTAO HOU** won a poster prize at the WONTON conference 6<sup>th</sup> Workshop on NanoTube Optics and Nanospectroscopy at Banz Monastery in Germany in June 2015. Her poster title was: “Defect-Dependent Brightening of Individual Single-Walled Carbon Nanotubes” and was co-authored with Dr. Sanela Lampa-Pastirk and advisor Professor Todd Krauss.



*Zhentao Hou with MIT Professor Millie Dresselhaus and another poster winner.*



*Amanda Preske receiving a poster award from Dr. Victor Klimov.*



Congratulations to Boeckman group member **DOUG TUSCH** and his wife Chelsea on the birth of their first child Tessa, born on May 27, 2015.

**LEAH FRENETTE** traveled to Swaziland in June 2015 as part of the NSF IGERT (Integrative Graduate Education Research and Traineeship) program with

five other U of R graduate students, including **MILES MARNELL** from the Jones lab. During the three weeks they were there, they visited five high schools to demonstrate scientific processes related to renewable energy and also taught a workshop on building solar panels. They taught over 850 students and helped them build more than 20 solar panels. They presented their research to the faculty at the University of Swaziland and traveled to Cape Town, South Africa for the PowerGen Africa Conference on the future of energy in southern Africa. Leah and the other graduate students had a tremendous experience.

The IGERT program has had 5 cohorts of students and is in its fifth, and final, year. Past chemistry students to win the fellowship include: Dr. Lenore Kubie (Krauss), Dr. Chris Favaro (Rothberg/Teng), and Amanda Preske (Krauss). Mike Mark from the McCamant group is in the final cohort and will travel to Swaziland in May 2016.





# Doctoral Degrees Awarded in Chemistry

From July 2014 through August 2015

## Stanislav Bellaousov

*Improving and Applying RNA Secondary Structure Prediction*

Advisor: David H. Mathews

## Peter N. Carlsen

*Synthesis of Tetrapetalone A-Me Aglycon*

Advisor: Alison J. Frontier

## Jonathan Chen

*Two- and Three-Dimensional Modeling of RNA Structure with NMR and Thermodynamics Methods*

Advisor: Douglas H. Turner

## David Condon

*Nucleic Acid Force Fields Used in Prediction of Ensemble NMR Properties*

Advisor: Douglas H. Turner

## Barbara Dunlap

*New Methods in Two-Dimensional Femtosecond Stimulated Raman Spectroscopy*

Advisor: David McCamant

## John Frost

*Methods and Reagents for the Post-Translational Cyclization of Genetically Encoded Polypeptides*

Advisor: Rudi Fasan

## Eric Henry

*A Study of Primary Collision Dynamics in Inverse-Kinematics Reaction of  $^{78}\text{Kr}$  on  $^{40}\text{Ca}$  at a Bombarding Energy of 10 MeV per Nucleon*

Advisor: Wolf-Udo Schröder

## Steven D. Jacob

*1, 6-Conjugate Addition Initiated Cyclization Reactions of Dienyl Diketones; Development of a Scalable, Divergent Synthetic Route to (-)-Rocaglamide*

Advisor: Alison J. Frontier

## James Kovach

*Electrophilic C-H Activation Using a Rhodium Diimine Complex*

Advisor: William D. Jones

## Lenore Kubie

*Metallopeptides and Metallocytochromes c with Single-Walled Carbon Nanotube Conjugates for Alternative Energy Applications*

Advisor: Kara L. Bren

## Wathsala G.H.M. Liyanage

*Amyloid-Inspired Amino Acid Based Functional Hydrogel Materials: Structural Insights*

Advisor: Bradley Nilsson

## Yekaterina Lyubarskaya

*Tuning Surface Properties Using Self-Assembled Monolayers for Various Applications*

Advisor: Alexander Shestopalov

## Elena Nilosek

*Quantum and Classical Molecular Dynamics of Energy Harvesting*

Advisor: Oleg Prezhdo

## Gregory A. Pilgrim

*Electrons, Protons, and Solvents in Carbon Nanotubes*

Advisor: Todd D. Krauss

## Fen Qiu

*Semiconductor Nanocrystals for Photocatalytic Hydrogen Production*

Advisor: Todd D. Krauss

## Randy Sabatini

*Excited State Dynamics, Molecular Interactions, and Electron Transfer in Systems for the Photochemical Production of Hydrogen*

Advisor: Richard Eisenberg

# Doctoral Degrees Awarded in Chemistry (continued)

*From July 2014 through August 2015*

## Terrell Samoriski

*The Design, Implementation and Evaluation of Peer-Led Team Learning (PLTL) in a Second Semester Organic Laboratory Course*

Advisor: Joseph Dinnocenzo

## Jessica Smith

*Macrocyclic Organo-Peptide Hybrids (MOrPHs): Methodology and Application Toward the Inhibition of Protein-Protein Interactions*

Advisor: Rudi Fasan

## Ria J. Swanekamp

*Understanding the Fundamental Mechanisms That Drive Amphipathic Peptide Self-Assembly*

Advisor: Bradley Nilsson

## Hui Wang

*Studies Towards the Total Synthesis of (-) - Nakadomarin A*

Advisor: Robert K. Boeckman, Jr.

## Kristina Wilson

*An Attempt at Direct Observation of Anharmonic Vibrational Coupling Constants with Two-Dimensional Femtosecond Stimulated Raman Spectroscopy*

Advisor: David McCamant



*Genessee River in Winter*

# Postdoctoral Fellows

## Albert Collins Nganou Assonkeng

Prof. McCamant (2012)  
Technical University, Berlin, Germany

## Priyanka Bajaj

Prof. Fasan (2014)  
National Institute of Pharmaceutical  
Education and Research, Mohali, India

## Sarina Bellows

Prof. Jones (2014)  
University of Rochester, Rochester, NY

## Nina Bionda

Prof. Fasan (2013)  
Florida Atlantic University, Boca Raton, FL

## Lipeng Chen

Prof. Franco (2008)  
Institute of Chemistry, Chinese Academy of  
Sciences, Beijing, China

## Sumit Chakraborty

Prof. Jones (2012)  
University of Cincinnati, Cincinnati, OH

## Simone Giovanni

Prof. Fasan (2014)  
Università di Siena, Siena, Italy

## Nicholas Gower

Prof. Weix (2012)  
University of Bristol, Bristol, UK

## Cassandra Hayes

Prof. Jones (2013)  
Simon Fraser University, Burnaby, Canada

## Eric Henry

Prof. Schröder (2015)  
University of Rochester, Rochester, NY

## Scott Hicks

Profs. Eisenberg and Krauss (2014)  
Purdue University, West Lafayette, IN

## Arnab Kar

Prof. Franco (2014)  
University of Rochester, Rochester, NY

## Peter Lamberg

Prof. Bren (2013)  
Malmö University, Malmö, Sweden

## Elzbieta Lenartowicz

Prof. Turner (2014)  
Polish Academy of Sciences, Poznan, Poland

## Corinne Minard

Prof. Frontier (2014)  
Ministère de l'Enseignement Supérieur et de la  
Recherche, Paris, France

## Salvadore Munoz

Prof. Neidig (2015)  
University of Indiana, Bloomington, IN

## Vijayadas Kuruppanthara Neelakandadas

Prof. Fasan (2014)  
CSIR-National Chemical Laboratory, Pune,  
India

## Phuong Quoc Thuc Nguyen

Prof. Fasan (2013)  
Nanyang Technological University, Singapore

## Linsen Pei

Prof. Farrar (1999)  
University of Science and Technology of  
China, P.R., China

## Purnima Thanthirige Ruberu

Prof. Eisenberg (2013)  
Iowa State University, Ames, IA

## Gopeekrishnan Sreenilayam

Prof. Fasan (2011)  
University of Iowa, Iowa City, IA

## Vikas Tyagi

Prof. Fasan (2013)  
CSIR-Central Drug Research Institute - Jawahar  
Lal Nehru University, India

## AUGUST 2014

### Lenore Kubie (University of Rochester)

“Metallopeptides and Metallochromes c with Single-Walled Carbon Nanotube Conjugates for Alternative Energy Applications” August 4, 2014

### Ria J. Swanekamp (University of Rochester)

“Understanding the fundamental mechanisms that drive amphipathic peptide self-assembly” August 8, 2014

### Yekaterina Lyubarskaya (University of

Rochester) “Tuning Surface Properties Using Self-Assembled Monolayers for Various Applications” August 8, 2014

### Stanislav Bellaousov (University of Rochester)

“Improving and Applying RNA Secondary Structure Prediction” August 12, 2014

### Kristina Wilson (University of Rochester)

“An Attempt at Direct Observation of Anharmonic Vibrational Coupling Constants with Two-Dimensional Femtosecond Stimulated Raman Spectroscopy” August 14, 2014

## SEPTEMBER 2014

### Amanda Preske (University of Rochester)

“Size-Programmed Synthesis of Lead Selenide Quantum Dots” September 3, 2014

### Professor Aaron Sadow (Iowa State University)

“Oxazolonylborate Metal Compounds and Catalysis” September 8, 2014

### Professor Aaron Esser-Kahn (University of

California - Irvine) “Chemical Biology Approaches to Innate Immunity and Vaccines: Probing a Code Without a Key” September 12, 2014

### Professor Angel Rubio (Universidad del Pais

Vasco - Spain) “Modeling non equilibrium dynamical processes in TDDFT: optoelectronic and photovoltaic applications” September 15, 2014

### Professor Masao Ikeda-Saito (Tohoku

University - Japan) “A New Way to Degrade Heme: IsdG-like Enzymes Degrade Heme without Release of CO” September 17, 2014

### Professor Steven Corcelli (University of

Notre Dame) “Solvation Dynamics and Vibrational Spectroscopy in Ionic Liquids” September 22, 2014

### Professor Jennifer Schomaker (University

of Wisconsin) “Oxidative Allene Amination in the Synthesis of Complex Molecular Scaffolds” September 26, 2014

### Professor Wesley Bernskoetter (Brown

University) “Carbon Dioxide-Olefin Coupling at Zerovalent Metals: Routes Toward Acrylates” September 29, 2014

## OCTOBER 2014

### Professor Adrian Roitberg (University of

Florida) “Underlying Thermodynamics of pH-Induced Allostericity: Is it Time to Stop Blaming the Poor and Overworked Histidines?” October 1, 2014

### Professor Zachary Tonzetich (University

of Texas - San Antonio) “Non-Traditional Organometallic Chemistry: Fundamental Studies and Catalytic Applications” October 6, 2014

### Professor Abigail Doyle (Princeton

University) “Methods and Mechanism in Asymmetric Catalysis” October 10, 2014

### Professor Mohammad A. Omary (University

of North Texas) “Advanced Functional Materials Made Smart for a “Spectrum” of Energy, Environmental, and Biomedical Applications” October 16, 2014

### Professor Mark Tuckerman (New York

University) “Materials in silico: Theoretical studies of structure and transport” October 22, 2014

### John Robert Frost (University of Rochester)

“Methods and reagents for the post-translational cyclization of genetically encoded polypeptides” October 23, 2014

### Professor Takashi Matsuo (Nara Institute

of Science and Technology) “Construction of artificial proteins based on complementary genetic and synthetic approaches” October 24, 2014

**Dr. Alexandre Tkatchenko (The Fritz Haber Institute of the Max Planck Society)** “The Many-Body Path Towards Predictive Modeling of Molecules and Materials” October 27, 2014

**Professor Paul Floreancig (University of Pittsburgh)** “Oxidative Carbocation Formation in Complex Molecule Synthesis” October 29, 2014

## NOVEMBER 2014

**Professor Neepa Maitra (Hunter College of the City University of New York)** “Electron Dynamics in Strong and Weak Fields: Landscapes of Steps and Peaks” November 3, 2014

**Professor Kevin Brown (Indiana University)** “Development of New Methods and Strategies for Stereoselective Chemical Synthesis” November 6, 2014

**Professor Michael J. Zdilla (Temple University)** “Synthetic Exploration of Unchelated Manganese Clusters of Reduced Coordination Number: A reinvention of Photosynthetic Water Oxidation Models” November 10, 2014

**Professor Valeria Molinero (University of Utah)** “Crystallization of water: a molecular perspective” November 12, 2014

**Barbara Dunlap (University of Rochester)** “New Methods in Two-Dimensional femtosecond stimulated Raman spectroscopy” November 14, 2014

**Dr. John Anderson (Northwestern University)** “Molecules to Materials: Synthetic Iron Compounds as Constructs to Explore Biological Systems” November 20, 2014

**Dr. Robert DiStasio (Princeton University)** “First Principles Approaches for Intermolecular Interactions: From Gas-Phase Dimers to Liquid Water and Molecular Crystal Polymorphism” November 24, 2014

## DECEMBER 2014

**Dr. Jeffrey McMahon (Northwestern University)** “From Shining Light on the Nanoscale to Taking Materials to the Extreme” December 1, 2014

**Steven D. Jacob (University of Rochester)** “1,6-Conjugate Addition Initiated Cyclization Reactions of Dienyl Diketones; Development of a Scalable, Divergent Synthetic Route to (-)-Rocaglamide” December 4, 2014

**Dr. Margaret Scheuermann (University of Washington)** “Cobalt-Catalyzed Alkene Hydroboration and Oxygen-Promoted C-H Activation at Palladium” December 4, 2014

**Dr. Helen Van Aggelen (Princeton University)** “How to model strongly correlated systems? The quandary of the universal method for quantum simulation” December 8, 2014

**Dr. Pengfei Huo (California Institute of Technology)** “New Theoretical Approaches to Simulate Exciton Transfer, Charge Separation, and Proton Reduction” December 11, 2014

**Dr. Gaël Ung (California Institute of Technology)**

“Carbene Chemistry: From Bond Activation to Dinitrogen Reduction” December 15, 2014

**Fen Qiu (University of Rochester)** “Semiconductor Nanocrystals for Photocatalytic Hydrogen Production” December 16, 2014

**Dr. Ellen Matson (University of Illinois at Urbana-Champaign)** “Design and Synthesis of Metalloenzyme Mimics for Nitrite Reduction” December 18, 2014

## JANUARY 2015

**David Condon (University of Rochester)** “Nucleic Acid Force Fields Used in Prediction of Ensemble NMR Properties” January 5, 2015

**Dr. Jonathan Foley (Argonne National Laboratory)** “Looking out for the tiniest lights: Controlling light at nanoscale dimensions for chemical applications” January 5, 2015

**Dr. Tzu-Pin (TP) Lin (California Institute of Technology)** “Boryl-Mediated H<sub>2</sub> Activation at Metal Centers: Applications in Catalysis” January 8, 2015

**James Kovach (University of Rochester)**  
“Electrophilic C-H Activation Using a Rhodium Diimine Complex” January 9, 2015

**Dr. Kathryn Knowles (University of Washington)**

“The Ins and Outs of Semiconductor Nanocrystals: How Core Composition and Surface Chemistry Control Function” January 12, 2015

**Dr. Lu Wang (Stanford University)** “Quantum Fluctuations in Hydrogen Bond Networks” January 15, 2015

**Peter N. Carlsen (University of Rochester)**  
“Synthesis of Tetrapetalone A-Me Aglycon” January 20, 2015

## **FEBRUARY 2015**

**Hui Wang (University of Rochester)**

“Studies Towards the Total Synthesis of (-)-Nakadomarin A” February 19, 2015

## **MARCH 2015**

**Professor Ivan Korendovych (Syracuse University)**  
“De Novo Design of Catalytic Function” March 13, 2015

### **W. Albert Noyes Jr. Memorial Lecture**

**Professor Louis Brus (Columbia University)**  
“Colloidal Semiconductor Nanocrystals -- History and Perspectives” March 16, 2015

“Strong Electron Correlation in Chemistry and Nanoscience” March 17, 2015

“Molecules Interacting with Plasmons - Single Molecule Raman and Charge Transfer Photochemistry” March 18, 2015

**Dr. Sergei Tretiak (Los Alamos National Laboratory)** “From engineering interfaces in soft electronic materials to efficient perovskite photovoltaics” March 27, 2015

**Elena Nilosek (University of Rochester)**  
“Quantum and Classical Molecular Dynamics of Energy Harvesting” March 27, 2015

**Professor Chong Fang (Oregon State University)** “Elucidating Photochemical Reaction Pathways in Fluorescent Protein based Biosensors using Ultrafast Spectroscopy” March 30, 2015

## **APRIL 2015**

**Professor Karen I. Goldberg (University of Washington)** “Catalysis, Mechanistic Understanding and Collaboration as Tools to Sustainable Production of Chemicals and Fuels” April 1, 2015

**Kierra Huihui (University of Rochester)** “Gold-Catalyzed Transformations of Alkynyl Aryl Sulfoxides” April 3, 2015

**Professor Mary Watson (University of Delaware)** “Transition Metal Catalysis of Non-traditional Electrophiles” April 6, 2015

**Professor Gregory H. Robinson (University of Georgia)** “Carbene-Stabilized Main Group Allotropes: Synthesis, Structure, and Reactivity” April 8, 2015

**Professor Suzanne Bart (Purdue University)**  
“Exploring the Role of Redox-Active Pyridine(diimine) Ligands in the formation of Uranium-Element Multiple Bonds” April 13, 2015

**Dr. Ke Chen (Bristol-Myers Squibb Pharmaceutical Company)** “Overcoming Steric and Electronic Obstacles: Development of Efficient Syntheses of Active Pharmaceutical Ingredients” April 17, 2015

**Randy Sabatini (University of Rochester)**  
“Excited State Dynamics, Molecular Interactions, and Electron Transfer in Systems for the Photochemical Production of Hydrogen” April 21, 2015

## Hutchison Memorial Lecture

**Professor Fraser Armstrong (Oxford University)** “The Discovery of Enzymes as Reversible Electrocatalysts - Implications for Designing the Energy Catalysts of the Future” April 21, 2015

“The Chemistry of Biohydrogen” April 22, 2015

“Enzymes in Solar Fuel/Artificial Photosynthesis Research” April 23, 2015

**Danielle Raymond (University of Rochester)** “Synthetic Molecular Machines” April 24, 2015

**Wathsala G.H.M. Liyanage (University of Rochester)** “Amyloid-inspired amino acid based functional hydrogel materials: structural insights” April 27, 2015

**Professor Andrew White (University of Rochester)** “New Methods for Combining Experimental Data and Molecular Simulations into Hybrid Models” April 27, 2015

## MAY 2015

**Lifeng Xiao (University of Rochester)** “Metal-Catalyzed Asymmetric 1,3 Dipolar[6+3] Cycloaddition of Azomethine Ylides” May 1, 2015

## Harrison Howe Award Lecture

**Professor David W. C. MacMillan (Princeton University)** “The Application of Photoredox Catalysis to New Transformations in Chemical Synthesis” May 7, 2015

**Gregory Arthur Pilgrim (University of Rochester)** “Electrons, Protons, and Solvents in Carbon Nanotubes” May 13, 2015

## Seymour Rothchild Lecture

**Professor Erick Carreira (ETH Laboratory of Organic Chemistry)** “Recent Advances in Asymmetric Catalysis” May 13, 2015

**Professor Art Bragg (Johns Hopkins University)** “Structural dynamics and heterogeneities of localized excited states in conjugated polymer materials” May 18, 2015

**Sarah J. Paulson (University of Rochester)** “Studies of the Catalytic Mukaiyama Aldol Reaction Utilizing Chiral Oxazaborolidines: Application to the Synthesis of Substituted Butenolides” May 20, 2015

**Terrell Samoriski (University of Rochester)** “The Design, Implementation and Evaluation of Peer-Led Team Learning (PLTL) in a Second Semester Organic Laboratory Course” May 26, 2015

**Jon Chen (University of Rochester)** “Two- and three-dimensional modeling of RNA structure with NMR and thermodynamics methods” May 27, 2015

**Miles Wilklow-Marnell (University of Rochester)** “Advances in Metal Mediated Conversion of Lignin to Value Added Products” May 27, 2015

**Professor Cynthia Burrows (University of Utah)** “Spirocycles and G-Quadruplexes: How the Chemistry of Guanine Oxidation Changes the Biology of DNA” May 28, 2015

## JUNE 2015

**Felipe Angel (University of Rochester)** “Novel Approaches to Increase the Performance of Organic Photovoltaic Devices” June 10, 2015

## JULY 2015

**Hsiu-Ying Wei (University of Rochester)** “Colloidal Semiconductor Quantum Dots with Tunable Surface Composition” July 15, 2015

**Eric Henry (University of Rochester)** “A Study of Primary Collision Dynamics in Inverse- Kinematics Reaction of  $^{78}\text{Kr}$  on  $^{40}\text{Ca}$  at a Bombarding Energy of 10 MeV per Nucleon” July 16, 2015

# Staff News

## ADMINISTRATIVE STAFF

The staff enjoyed their annual summer outing at a Red Wings baseball game in July.



**DEB CONTESTABILE** is in her fourth year with the Chemistry Department. As the Course Administrator, she works with faculty and the Registrar's office to schedule and plan all chemistry courses and related matters. In her role as the Undergraduate Program Coordinator, Deb serves as a member of the Chemistry Undergraduate Studies Committee (USC), helping students declare their major/minor, plan their program of studies, or receive transfer credit. Other responsibilities include setting up visits with prospective students, coordinating various meetings and events (including departmental Commencement related events), and working with student employees to help maintain the departmental website. In addition, she is also CLASP certified and will be assisting with pre-grant proposals. Outside of work, it's been an exciting year for Deb, her husband, and their two boys. Her oldest son graduated from high school, and recently started college life at R.I.T.



**ROBIN COOLEY**, our graduate studies coordinator, has been with the department for over ten years. Her duties involve coordinating departmental recruitment and admission activities, as well as assisting current students as

they progress through their studies toward the doctoral degree. Each year, Robin organizes the department's main recruitment activity, Visitation Weekend, which draws prospective graduate students from all over the US to experience Rochester and all that the department has to offer. This past year the attendees were welcomed with a night of fun and games at the Strong Museum of Play hosted by the current graduate students, followed by a full day of activities including tours, faculty talks and socializing. The event concludes with a reception and dinner event held at the Rochester Museum & Science Center. Each fall, Robin also organizes a week long orientation event for all incoming graduate students. For the 2015-2016 school year, we welcomed nineteen new graduate students to the department.

**DONNA J. DOLAN** is currently beginning her twenty-eighth year in Chemistry serving as departmental receptionist and purchaser. In this role, Donna continues to provide support for purchasing in the Chemistry Business Office while also providing assistance to faculty and managing the chemistry department's main office. In addition, she organizes the departmental distinguished lecturer's program. Donna continues to enjoy riding her XL883 Harley.



**GINA EAGAN** is the administrative assistant to Professor Lewis Rothberg, chair of the Materials Science program. With the addition of two Ph.D. and eight M.S. students this fall, there are a total of 21 Ph.D. and 17 M.S. students in the program. Some of Gina's responsibilities include explaining the graduate requirements to students and faculty, assisting with course registration and exam scheduling, and



working closely with the Graduate Studies office and ISO to submit all of the required documentation. Gina and her family love to participate in outdoor activities during all of the seasons. As a native of Rochester, she

encourages her two children to dress for the weather and go outside and have fun!!



**LYNDA W. MCGARRY (M.S. '85)**, completing her fifth year with the department and finishing up her second year as the Development and Alumni Relations Administrator, enjoys working with faculty on preparing grants and awards submissions, as well as organizing alumni and department events. Lynda, her husband Dan, and their family like to get away to their cottage on Port Bay, which is a few miles east of Sodus Bay, as often as possible. They enjoy going on the jetski and boat in the summer or snowmobiling in the winter. Their son Ian is a sophomore at SUNY Oswego, and their daughter Claire just started a new position as a data analyst at the NY State Department of Health in Albany after obtaining an M.S. in Public Health and Epidemiology from SUNY Albany. They are all hopelessly optimistic Buffalo Bills fans!



**KATE REINHARDT** is finishing her third year in the chemistry department. Kate and Elly work together in prepping the undergrad labs as well as shipping and receiving for the department. Kate distributes dry ice and gas cylinders, and is responsible for inspecting the research labs for safety compliance. She is completing her Masters in Business Administration at the Simon School of Business in May. Besides taking classes part-time and working in the department, she teaches kickboxing classes for U of R Intramurals at the River Campus Gym and is involved in both a basketball and kickball league!



**KENNETH SIMOLO (PH.D. '85)** starts his twenty-eighth 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.

**BARBARA SNAITH** completed her fourth year with us on July 1st as Administrative Assistant to the Chair of the Department. Barb continues to be a great asset to our Department and enjoys her many responsibilities, including organizing faculty recruiting, attending monthly faculty meetings and preparing the discussion minutes. She also organizes annual staff outings and holiday lunches for the department. Barb also manages the immigration paperwork needed for the Department's incoming Research Postdoctoral Associates as well as visiting students and professors, many of whom are foreign nationals. In her spare time, Barb enjoys fundraising for Lollypop Farm and supporting organizations such as the American Cancer Society, Natalie's Wings (organization that supports people with paralysis) and the Upstate Multiple Sclerosis ("MS") Society. She continues to attend GEVA theater productions and Rochester Broadway Theatre League plays with her good friends. Barb is also a captain of a volleyball team that has been playing for years and continues to be active by attending several jazzercise classes every week! She is still a very active member of her church, chairing fundraisers and women's events. In early October, Barb's 17 year old kitty, Snowball, passed away suddenly. He will be missed!! But, some good news, in December, Barb adopted two kittens that are sisters, Lily and Annabelle, from Lollypop Farm and has shared their photo with Santa.



**MARGUERITE WESTON**, assistant to faculty, has been with the Department of Chemistry for nineteen years. She coordinates Chemistry's seminar program by scheduling rooms, contacting speakers to ensure their travel arrangements are in place, obtains their titles and abstracts, prepares schedules of visits with department faculty, along with producing and advertising the online seminar schedule each month throughout the University community. Marguerite also coordinates select special events, assists with various projects, and provides support to numerous faculty members. She assists Professor Thomas Krugh with the many administrative details of Chemistry's National Science Foundation supported annual summer research program for undergraduates (REU). The program attracts approximately 100 applications each year from undergraduates across the nation and the University of Rochester. Marguerite and husband, Art, are residents of Henrietta, NY, enjoy dancing and gardening and have 3 sons and five grandchildren (plus 2 cats!).

**ELLY YORK**, who joined the chemistry department in November of 2006, works part-time prepping for the undergraduate general chemistry laboratories. Elly also assists part-time in the chemistry stockroom. Elly is a graduate of Alfred University and has a Master's degree in education. She also has clinical experience, having previously worked in several veterinary clinics prior to coming to the UR. On July 8th, Elly and her husband, Brandon, celebrated their son Aaron Timothy's fourth birthday, and on August 21st son Caleb Noah's first birthday. The family has enjoyed many outings this summer, like this one to the Great Balloon Rally in Wellsville, NY.



## THE EDITORIAL OFFICES

**VALERIE DRAKE** has been working for the past two years with Prof. Kara L. Bren as Editorial Assistant with the *Journal of the American Chemical Society (JACS)*. Val received her M.S. in Biology from University of Rochester, and finds her position as Editorial Assistant to be continually fascinating. Val and her husband, Lee, are both mentors for Penfield High School's FIRST robotics team 1511, "Rolling Thunder." Their son, Calvin, recently moved back to Rochester after graduating from USC, and has accepted a position as a video game developer with a local company. The photo shows Val enjoying a catamaran sailboat ride in the Caribbean.



**VALERIE FITZHUGH** has been working as an editorial assistant in the Department of Chemistry for almost thirteen 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. Val's passion is her family, especially her three grandsons, and she hopes to be retiring in the not too distant future so that she can spend more time with them, and with her ever growing gardens.

We are always delighted when **MARINA TOKINA**, journal assistant to her husband, former UR professor Oleg Prezhdo, stops by for lunch and dessert with the staff.



**TERRELL SAMORISKI** began her eleventh year working for *The Journal of Organic Chemistry (JOC)* this August, 2015. Since completing her PhD requirements she now works remotely with the JOC Chief-Editorial-Office in Salt Lake City, Utah and enjoys her new job requirements as an Assistant Research Data Analysts. Her first introduction to scientific publication was as a structure editor for the Chemical Abstract Service, which she was able to visit in her new role. As a direct result of the contributions of the JOC Editors and staff, the Thomson Reuters Impact Factor for 2014 increased to 4.721 and again set a new standard with 101,519 total citations.

## SCIENTIFIC & TECHNICAL STAFF

**BILL BRENNESEL** continues to manage the X-ray Crystallographic and CENTC Elemental Analysis facilities. With single crystal X-ray diffraction, only one crystal (like a sugar or salt crystal, but generally of something new and exciting) of a batch is examined. While this technique offers exemplary characterization of that crystal, providing us with atomic bond lengths and angles, as well as the 3D arrangement of the molecule among the tens of thousands of others within the crystal, it is truly only valid for the one crystal that was examined. This is where the second technique—elemental analysis—comes into the picture. This form of characterization is performed on the bulk sample, thus independently confirming (or not!) that the result from the X-ray experiment is representative of the entire sample. During the spring semester Bill also teaches the graduate course in X-ray crystallography (CHM 416) as well as devotes a week to CHM 234 students to introduce them to the technique. Both courses include a combination of theory and hands-on training. As an additional incentive, students who successfully complete CHM 416 become officially trained users of the X-ray facility and are authorized to independently operate the equipment for their own research. Throughout the year Bill collaborates with

various professors from the local colleges, most recently with Professor Bradley Kraft from St. John Fisher College and Professor Carly Reed from the SUNY College at Brockport. Bill is very generous with his time and cooking skills as he mans one of the two grills outside Hutchison Hall at lunchtime every Tuesday throughout the year no matter what the weather brings. We are all grateful to Bill and the entire Tuesday Grill Team of Ted O'Connell and Ray Teng, for providing tasty food at a very reasonable price and always with a smile!

**TERRY (TED) O'CONNELL** has completed his 32nd year at the University of Rochester in the Department of Chemistry as the Supervisor of the Department's Technical staff, Mass Spectrometers, and taking care of the hardware maintenance of departmental instrumentation. On the weekends, both he and Marlene, his significant other, continue to enjoy weekend motorcycle rides and playing with Benjamin and Scuffy, two rescued beautiful Airdale terriers!

**SUE CARDINAL**, Chemistry Librarian from the Carlson Library, reports that she holds office hours in the Chemistry department on Monday mornings and Friday afternoons. The Library has purchased the Taylor and Francis Journal Archive. There have been four staff changes as people retire or move on to school or new positions. We are learning about electronic laboratory notebooks to see if they have a place at Rochester. The Carlson Library has begun to add programming and services on the first floor to support undergraduate research experiences.

**ERIC LOBENSTINE (PH.D. '81)**, manager for computers and network, reports another year of pretty smooth sailing for our computers and network, for which he is glad. He is currently working to transition the Chemistry email service to the University's service (Microsoft Office 365). He reports that it is not a lot of fun, but hopes that it will be worth it in the end. He continues to represent Chemistry's interests on several IT committees within the University; he routinely advises IT directors on how various University IT initiatives will be viewed at the department level - "in the trenches", so to speak. Eric's wife, Jeanne, has finished a year long sabbatical from her work as a physician, and is starting to work again, being mindful not to overextend herself. Her garden this year has been spectacular! Eric and Jeanne's sons, Brian and Ethan, continue sharing a house in Cambridge, MA. Ethan has just started a Masters degree program at New England Conservatory! Brian finds that owning a dog has really helped him cut back his long hours at work as a Customer Service Manager for Parker-Hannifin.



**JALIL SHOJAIE** is currently a Sr. lab engineer/chemist who works mornings in the chemistry department and afternoons at the University Laboratory for Laser Energetics (LLE). He has been at the University of Rochester since 1996. He worked as a research chemist in both the OB/GYN and anesthesiology departments. Prior to coming to Rochester, he worked as a research chemist at NYU, Nelson Institute of Environmental Medicine (1990-95). He has peer-reviewed research publications and patents, with both the University of Rochester and NYU.

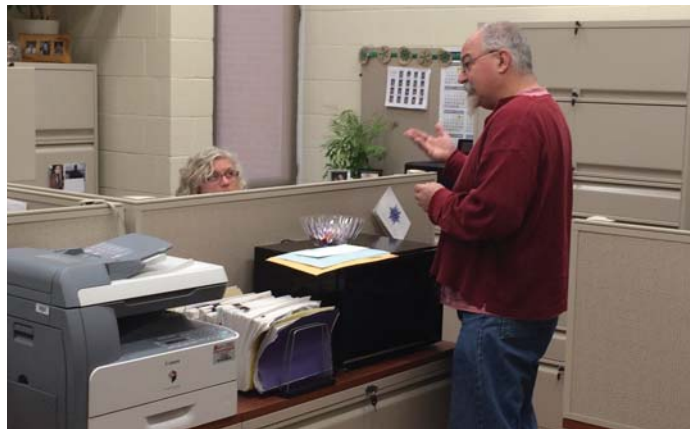
**RAY TENG (B.S. '83, M.S. '87, M.B.A. '01)** has been with the University since 1987 and joined chemistry in 2004 as research/facility coordinator. Ray brings many years of experience to the department, having previously worked in the Department of Physics and Astronomy, the Nuclear Structure Research Laboratory, and the Department of Earth and Environmental Sciences as senior technical associate. Ray continues to enjoy the daily interactions with faculty and students in addressing research and facilities issues, and he has been very busy with the renovation of the department's administrative offices. Ray's daughter Sydney graduated from Johns Hopkins, and was a member of their Division III soccer team which made it to the final 4 in her senior year. She is now working at a law firm in Washington, D.C. where his younger daughter, Addison, is in her second year at American University.

## THE BUSINESS OFFICE

The Business Office continues to provide service to faculty, staff and students on all financial matters such as payroll, reimbursements, purchases, preparation of grant budgets and monitoring grant expenditures. **DORIS WHEELER**, business office manager since 2002, is very happy to report that the business office is running smoothly. The business office staff consists of four members with valuable experience. **ANNA KUITEMS** is responsible for reconciling grant ledgers, P-card management and graduate student payroll, and as backup for Randi Shaw. A major change this year is UR Financials replaced the current legacy Financial Records System (FRS), the system that has been used for over 40 years to record the University's financial and accounting activities, with Workday Financials. The move to UR Financials using Workday, a cloud-based solution, will mitigate risk associated with the existing mainframe system, modernize finance and accounting services including built-in best practices, and create a more sustainable system architecture. The Business Office has been undergoing another change this year with a facelift to their offices with new flooring and furniture to their area.

**RANDI SHAW**, the chemistry accounting bookkeeper, is responsible for billing internal charges, purchase orders, reconciling ledgers, employee reimbursement forms, and processing invoices.

**DIANE VISIKO**, TAR accounting bookkeeper, continues to work with departmental payroll and is the "Timekeeper" for HRMS. With her flexible schedule, she is able to spend more time with her nine grandchildren.



**PAUL LIBERATORE** continues to provide exceptional service as the manager of the chemistry stockroom located in the basement of Hutchison Hall. Paul has been with us for 30 years now.

## INSTRUCTIONAL FACULTY

**BENJAMIN HAFENSTEINER** and his wife, Amanda Gorman, are busy keeping up with their one year old daughter Scarlett who was born on September 5, 2014. Ben received his Ph.D. from The Scripps Research Institute in 2008, and proceeded on to a postdoctoral fellowship at UC Irvine in Dr. Larry Overman's group. "Prof. H", as he is called by his students, has been an instructional faculty member for General and Organic Chemistry since 2011.



# Instrumentation

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

## NMR Spectrometers:

- ~ Varian 500 MHz Inova NMR Spectrometer
- ~ Brüker 500 MHz Avance NMR Spectrometer
- ~ Two Brüker 400 MHz Avance NMR Spectrometers
- ~ Brüker AMX 300 MHz NMR Spectrometer

## Mass Spectrometers:

- ~ Thermo Scientific LTQ Velos with Accela LC system
- ~ Brüker Autoflex III Smartbeam MALDI-TOF
- ~ Two Shimadzu GC/MS QP-2010 with EI,CI,-CI
- ~ Shimadzu LC/MS QP-2010, with APCI & ESI

## X-Ray Diffractometers:

- ~ A Siemens SMART CCD X-ray diffractometer with a SMART APEX CCD area detector
- ~ A KRYO-FLEX low temperature device.

## Photochemistry Facilities:

- ~ Radiant Dyes RD-EXC-200 excimer laser and Radiant Dyes NarrowScan dye laser for nanosecond transient absorption experiments.
- ~ Continuum high energy picosecond Nd:YAG laser (Leopard, model D-20).
- ~ Tunable, femtosecond Ti : Sapphire laser with harmonic

generator (second and third), and pulse selector coupled to a PicoQuant FluoTime 200 spectrometer and PicoHarp 300 time-correlated single photon counting module.

- ~ Time-resolved, single molecule fluorescence facility, included are: Femtosecond/Picosecond Ti:sapphire
- ~ Oscillator and Optical Parametric oscillator; 2 Avalanche Photodiodes (PicoQuant); Inverted optical microscope (Nikon TE 2000).
- ~ JY Horiba FL3-22 Fluorolog 3 spectrofluorometer equipped with double-grating excitation and emission monochromators.
- ~ Perkin-Elmer Lambda 35 UV-vis-NIR spectrophotometer with a spectral range of 190-1100 nm.



*Neidig Group member Jared Kneebone inserting his sample into the NMR*



*Organic Chemistry students in lab (J. Adam Fenster)*

### **Other Instruments Include:**

- ~ Shimadzu Model 8400-S Fourier Transform IR configured with a Pike MIRacle ATR sampling accessory - diamond window for analysis of solids, liquids, pastes, and gels.
- ~ Five Shimadzu FTIR Spectrometers
- ~ Remspec ReactionView IR spectrometer with ATR and transmission probes for in situ reaction monitoring.
- ~ Bruker ESP-300 ESR spectrometer.
- ~ See Co. MS4 Mössbauer spectrometer equipped with a Janis SVT-400  $L_{N_2}/L_{He}$  cryostat
- ~ Magnetic Circular Dichroism spectrometer with a spectral range of 190-2000 nm and temperature control from 1.6 K - 300 K.
- ~ Three potentiostats for electrochemistry from CH instruments
- ~ CENTC Elemental Analysis Facility at the University of Rochester (can handle even water- and oxygen-sensitive samples)
- ~ Bruker EMX-Plus EPR spectrometer with 4 K temperature Capability
- ~ CEM Explorer Microwave Synthesizer
- ~ Thales Nano H-Cube continuous-flow hydrogenation reactor
- ~ Perkin Elmer 2400 CHN/S Analyzer with VAC Atmospheres (Argon) glove box
- ~ Perkin Elmer Lambda 950 UV/VIS Spectrometer
- ~ Perkin Elmer Lambda 950 UV/VIS Spectrometer with Peltier temperature control unit
- ~ Shimadzu 6300 Atomic Absorption Spectrometer
- ~ Single-molecule time-resolved fluorescence confocal microscope
- ~ Thermogravimetric analysis and Differential Scanning Calorimetry for polymer characterization
- ~ Digital Instruments Nanoscope IIa Atomic Force Microscope
- ~ Ellipsometer
- ~ Spectrofluorometer from Roper Scientific, infrared and visible
- ~ Many UV-Vis spectrometers
- ~ Phosphoimager

# Departmental Funds

You may also donate online at: [www.chem.rochester.edu/alumni/giving.php](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 Fellowship awards to support graduate research and education, the purchase of undergraduate laboratory equipment, assisting graduate students with travel expenses to scientific conferences, and supporting Chemistry's outside speakers program. Note that this fund is under direct control of the Department, and allows Chemistry to expand the scope of its research and teaching activities as needed. By contrast, the "Dean's Fund for Chemistry" is under control of the Dean of the College and not the Department, and is primarily used to supplant the College's expenses for ongoing Chemistry activities.

## Richard Eisenberg Chemistry Endowment

A new fund named to honor the distinguished career contributions of Richard S. Eisenberg, the Tracy H. Harris Professor Emeritus of Chemistry. Our goal with the fund is to endow a Chaired Professorship that can be used to attract a senior hire in the areas of inorganic chemistry, photoinduced charge transfer and/or photochemistry. In addition to allowing the faculty size to more rapidly grow to our new allotment, the Chaired Professorship position will allow us to build on current strengths in the Department in catalysis and photochemistry in order to nucleate larger, campus-wide research efforts in these areas.

### I wish to contribute to the following fund:

Chemistry Alumni Research Fund

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

My gift is in honor of \_\_\_\_\_ (see above)

### Contact Information:

NAME \_\_\_\_\_

ADDRESS \_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_  
\_\_\_\_\_

### Degree Information:

*Year degree(s) received from the Department*

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

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

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

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

ADVISOR \_\_\_\_\_

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







University of Rochester  
Chemistry Department  
Hutchison Hall, RC Box 270216  
Rochester, NY 14627-0216

