

William D. Jones

Charles F. Houghton Professor of Chemistry

Ph.D. 1979, California Institute of Technology



RESEARCH INTERESTS

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

CONTACT

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

carbon bond strengths that allows us to make predictions about stabilities. The group continues its role in the Center for Enabling New Technologies through Catalysis (CENTC), in which the group has collaborative research projects that are exploring new electrophilic C-H activation catalysts and new direct routes to aromatic amines from benzene. Bill continues as Associate Editor for the *Journal of the American Chemical Society* for an eighth year, where he handled close to 500 manuscripts last year. He lectured in/at Oviedo, Taiwan, Boston, Durham, Beijing, Lanzhou, Lyon, Hawaii, Chicago, Buffalo, Columbia U., Anaheim, Carleton College, Morocco, Montreal, and France. Two graduate students completed their degrees, **TING LI (PH.D. '10)**, and **MATT GROCHOWSKI (PH.D. '10)**. Ting is now with DuPont in Shanghai, and Matt is doing a postdoc at Penn. St. with Ayusman Sen. Bill

Bill Jones in Errachidia, Morocco



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

The group's scientific accomplishments have centered upon our work in alkane C-H bond activation, in which we showed that a rhodium complex first binds to an alkane and then cleaves the C-H bond. Studies have shown that the metal will only break the C-H bonds in the terminal methyl groups. This selective feature was also surprisingly seen in the activation of 1-chloroalkanes and 1-cyanoalkanes. Investigations of competitions between various nitriles show a preference based on chain length, consistent with the notion that the metal binds to the chain and then 'walks' down to the end before inserting. With chloroalkanes, the opposite is seen, i.e., all chain lengths compete 1:1. This led to the postulate that binding to the chlorine was rate determining, not the binding to the alkyl chain. Using kinetic techniques, it was determined that a rhodium-methyl bond is 3 kcal/mol stronger than a rhodium-cyanomethyl bond, yet C-H activation adducts of the latter are more stable because reductive elimination leads to the formation of a weaker C-H bond. This analysis is being applied to other substrates to come up with a global understanding of C-H activation thermodynamics and metal-carbon bond strengths.

Our work in C-H activation is also continuing in a collaborative research effort in the Center for Enabling New Technologies through Catalysis (CENTC). This NSF-funded center

includes researchers from a dozen universities participating in joint projects and using cyber-conferencing to discuss results. This mode of research is testing a new paradigm for conducting research and following the first successful three year initiation, the Center was fully funded with \$15M to support activities over a five year period, and will be up for renewal this fall. Our group is also continuing mechanistic work on C-CN cleavage. We have determined that in C-CN cleavage of benzonitriles, coordination to the arene, not the nitrile, precedes bond cleavage. Detailed DFT studies have been used to support this pathway, and a novel migratory process of the metal has been elucidated. The group also continues its collaborative work on C-CN cleavage with Professor Juventino Garcia at the Universidad Nacional Autonomas de México.

Bill has also been invited back to China this fall to speak at the meeting of the State Key Laboratory of Elemento-Organic Chemistry in Tianjin. He will also speak at the ISHHC in Berlin and at the Spanish Meeting of Organometallic Chemistry in Castellon. He is also a member of the International Scientific Committee for the International Conference on Organometallic Chemistry 2012. The group is supported by continuing funding from the Department of Energy, the National Science Foundation, and the NSF Center Enabling New Technologies through Catalysis.

Andrew S. Kende

Charles F. Houghton Professor Emeritus of Chemistry

Ph.D. 1957, Harvard University



RESEARCH INTERESTS

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

CONTACT

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

Rush Rhees Library Detail





RESEARCH INTERESTS

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

CONTACT

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

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

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





Goergen Hall

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

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

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

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

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

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

Robert W. Kreilick

Professor Emeritus of Chemistry

Ph.D. 1964, Washington University



RESEARCH INTERESTS

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

CONTACT

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ROBERT KREILICK is enjoying his fourth year as Professor Emeritus of Chemistry. Professor Kreilick's research involves investigations of magnetic and electrical properties of solid transition metal complexes and organic free radicals. Experiments which produce information about electron-electron exchange interactions, dipolar interactions, and electrical conductivity are conducted. Three years ago, new software was written for the ESR spectrometer and low temperature equipment was brought back into working order. We now have an ESR center which is being used by other chemistry faculty members.



Finger Lakes View

Thomas R. Krugh

Professor of Chemistry

Ph.D. 1969, Pennsylvania State University



RESEARCH INTERESTS

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

CONTACT

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

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



David W. McCamant

Assistant Professor of Chemistry

Ph.D. 2004, University of California, Berkeley



RESEARCH INTERESTS

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

CONTACT

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

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

Memorial Art Gallery



John S. Muentner

Professor Emeritus of Chemistry

Ph.D. 1965, Stanford University



RESEARCH INTERESTS

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

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

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



John with grandson, Corey Edwards at nine months

Bradley L. Nilsson

Assistant Professor of Chemistry

Ph.D. 2003, University of Wisconsin, Madison



RESEARCH INTERESTS

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

CONTACT

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

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

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

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

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

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

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

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

Nilsson Group, Summer 2011



Oleg Prezhdo

Professor of Chemistry

Ph.D. 1997, University of Texas, Austin



RESEARCH INTERESTS

Theoretical physical chemistry with focus on dynamics in condensed phase, nanoscale and biological systems. Semiclassical theories, non-adiabatic molecular dynamics, time-dependent density functional theory, and related approaches are applied to problems in time-resolved spectroscopy, renewable energy harvesting and storage; nanoscale electronics and spintronics, and biological bonds.

CONTACT

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

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

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

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

Speegle-Wilbraham Aquatic Center in the Goergen Athletic Center





Eastman School of Music at night

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

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

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

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

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

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

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

Lewis J. Rothberg

Professor of Chemistry

Ph.D. 1983, Harvard University



RESEARCH INTERESTS

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

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

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

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

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

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





Wilson Commons

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

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

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

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

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

William H. Saunders

Professor Emeritus of Chemistry

Ph.D. 1952, Northwestern University



RESEARCH INTERESTS

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

CONTACT

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

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

Wolf-Udo Schröder

Professor of Chemistry

Ph.D. 1971, University of Darmstadt, Germany



RESEARCH INTERESTS

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

CONTACT

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

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

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

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

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

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

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

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



Udo in Berlin, Germany





RESEARCH INTERESTS

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

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

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

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

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



Douglas H. Turner

Professor of Chemistry

Ph.D. 1972, Columbia University



RESEARCH INTERESTS

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

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

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

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

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

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

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



Winter Scene at Mt Hope Cemetery

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

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

Daniel J. Weix

Assistant Professor of Chemistry

Ph.D. 2005, University of California, Berkeley



RESEARCH INTERESTS

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

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

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



Weix group member works in our newest glove box

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

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



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

Weix Group, Summer 2011

