

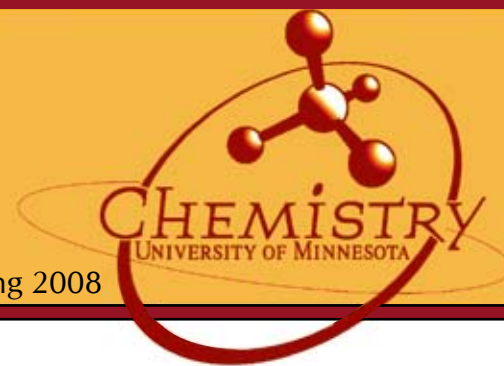


# ChemNews

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An Institute of Technology Department

Spring 2008



## GREETINGS FROM THE CHAIR



Jeff Roberts

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Dear Friends,

There is much to report in this year's newsletter, most of it good, but some sobering. On a sad note, we continue to mourn the death of our colleague Marian Stankovich last June. Although Marian can never be replaced, it is wonderful that in the midst of that terrible loss, the department welcomed three new assistant professors: Chris Douglas, Andy Harned, and Valerie Pierre. I know you'll be hearing a lot about them over the next few years. Also, Andy Taton was tenured and promoted to associate professor, and Marc Hillmyer was promoted to full professor.

The awards flowed in, as we have come to expect, to faculty members, graduate students, and undergraduates, including a Rhodes Scholarship to U of M chemistry and biochemistry major Katie Lee. In short, the department continues to grow and thrive, and to educate more and more chem-



ists who leave the department to make their own marks on the world. I think—in fact I *know*—that Minnesota-educated chemists rank among the nation's best.

As I reflect on the Chemistry Department, I cannot help but be as optimistic for the future as I am impressed by the past. We have an extraordinary department, built on a solid foundation of outstanding teaching, superb research, and wonderful people. But I assure you, the best is yet to come.

With warmest wishes,

### **University of Minnesota CHEMISTRY ALUMNI & FRIENDS BREAKFAST**

**Tuesday, April 8, 7:30 AM: Reservation #415**

**at the Spring 2008 American Chemical Society National Meeting & Exposition**

**Sunday, April 6 —Thursday, April 10, 2008, New Orleans, LA USA**

**UMN Professor Lawrence Que, Jr. is the recipient of the  
2008 Alfred Bader Award in Bioinorganic or Bioorganic Chemistry**

(see page 15)

## Lou Pignolet Receives President's Award for Outstanding Service 2006

**Lou Pignolet**, Institute of Technology Distinguished Professor, has been a faculty member in the Department of Chemistry for thirty-six years. Described as an innovator, a mentor, and a model citizen, Professor Pignolet has made outstanding contributions to teaching, research, and service. He has made a notable impact on science education in the state. In the 1970's, he created the Lando Summer Research Program, which brought sophomores and juniors from other institutions to spend a summer doing research at the University of Minnesota. He also was responsible for a summer program in chemistry created for Native American junior high school students and the Chemical Outreach Program, a program in which undergraduates in chemistry and related fields demonstrate chemical experiments to classrooms, scout troops, and family events. "Chem Day," another initiative he created, attracted more than 600 high school students and teachers annually. Not only have these programs brought publicity to the University, but have also taught kids that science is fun and interesting. He has served on numerous committees at the department, college, and University level, including the Graduate School Research Advisory Committee, the Special Committee on K-12 Education, the Student Judicial Affairs Committee, and the President's Distinguished Faculty Mentor Program. He is the recipient of several awards and recognition such as the Morse-Alumni Award for Outstanding Contributions to Undergraduate Education and has been named eight times "Best Chemistry Professor of the Year" by the IT Student Organization.



*Lou Pignolet receives award from UMN President Bruiniks*

## In Memoriam: Marian T. Stankovich

**Marian Stankovich**, a long-time professor of chemistry at the University of Minnesota, died suddenly on June 19, 2007. She was 59. Marian was an expert in bioanalytical chemistry studying the function of enzymes. She primarily used electrochemical methods to study enzymes in electron transfer reactions. Her research serves as a building block to understanding diseases in the human body, including Sudden Infant Death Syndrome.



She was often the go-to person on using electrochemical methods to study enzymes and collaborated with other researchers here at the University and around the world.

Stankovich came to the University in 1981, during a tumultuous time in its history. The University had just settled a class-action lawsuit to improve the climate for women faculty.

"She struggled in those early years against some with ingrained antipathy to the role of women in a chemistry department," said Pete Carr. "Marian persevered due to her love of science, her courage, persistence, single-mindedness and very hard work."

She became the first woman tenured in the Department of Chemistry, paving the way for future generations of women in science.

## Andreas Stein Becomes Merck Professor of Chemistry

Andreas Stein is the newest recipient of a named professorship in the Chemistry Department. On July 1, Andreas will begin a five-year term as a Merck Professor of Chemistry. The Merck Professorships (there are two of them; Kent Mann holds the other one) are funded through generous gift endowments to the Chemistry Department and matching funds from Permanent University Fund resources.

## Edgar Arriaga Receives University of Minnesota Fesler-Lampert Chair in Aging Studies

The Fesler-Lampert Chair was created in 1999 with support from the University of Minnesota Graduate School and the generosity of David and Elizabeth Fesler. The chair funds researchers and scholars who are conducting research in a project related to the subject of aging.

### Chemistry Promotions

Marc Hillmyer: to Professor

Andy Taton: to Associate Professor

## Three New Faculty Join Department

**Chris grew up on a mink farm** near Perham, Minnesota before attending middle and high school in Berlin, Wisconsin. He earned his Bachelor's of Science degree from the University of Minnesota-Twin Cities in 1999, working with Richard Hsung to develop new reaction methodologies. Chris earned his Ph.D. studying under Larry Overman at the University of California, Irvine. During his graduate studies, he worked on projects concerning the total synthesis of marine alkaloids and catalytic asymmetric sigmatropic rearrangements. Without leaving sunny southern California, Chris conducted his postdoctoral studies as an NIH-NRSA postdoctoral fellow with Robert H.

### Dr. Christopher J. Douglas

Grubbs at the California Institute of Technology in Pasadena investigating unreactive carbon-hydrogen bond activation and functionalization using rhodium porphyrin complexes.

Chris was excited to return to his alma mater to explore his research interests in organic synthesis and organometallic chemistry. His research group is exploring the uses of transition metal catalysts to activate carbon-carbon sigma bonds for new chemical transformations. The reactions discovered in his group could lead to more efficient syntheses of targeted molecules, such as natural products or drug candidates. Chris is also interested in the design and synthesis of new small-molecule semiconductors. He is particularly interested in using transition metal catalysts to access new compounds capable of self-assembly into well-defined 3-D structures to maximize charge transport.



### Dr. Valerie C. Pierre



**Valerie was born near Bordeaux, France** where she spent much of her childhood before moving to Edmonton, Canada at the other side of the globe at the age of ten. She returned to France for her undergraduate studies and obtained her Engineer's Diploma from the Ecole Supérieure de Chimie in Lyon, France in 2001. After a year of internship at BASF-AG in Ludwigshafen am Rhein, Germany, Valerie moved back to North America for graduate studies in chemistry at the University of California, Berkeley with Kenneth N. Raymond on the design, synthesis, and evaluation of gadolinium-based contrast agents for Magnetic Resonance Imaging. After obtaining her Ph.D. in 2005, Valerie moved to the California Institute of Technology for postdoctoral studies with Jacqueline K. Barton. While in Pasadena she elucidated, both by crystallography and by NMR, the structure of a novel binding mode of inert metal complexes with DNA.

Valerie is now joining the strong bioinorganic and bioanalytical teams of the Department of Chemistry at the University of Minnesota where her research group is developing metal complexes for use in probing biological and medical systems. Part of her research is directed at designing and synthesizing luminescent lanthanide-based sensors for the quantitative and spatial determination of biological analytes of interest such as nucleotides. Her group is also developing novel nanomaterials for use as highly sensitive and responsive contrast agents in Magnetic Resonance Imaging.

**Andy was born in Georgia** but, because of his military father, lived in five other states and one other country before settling in Woodbridge, VA. After three years in one high school, Andy went to Virginia Tech for a degree in biochemistry, but spent all of his research time in the chemistry department working in the laboratories of Profs. Neal Castagnoli and Michael Calter. In Kansas as a graduate student he worked under the guidance of Paul Hanson investigating the utility of ring-opening metathesis polymerization as a general purification tool for organic reactions. Upon completion of his degree, he continued his trek across the country

### Dr. Andrew M. Harned

and conducted work at Caltech in the labs of Prof. Brian Stoltz as an NIH postdoctoral fellow. His work at Caltech focused on enantioselective Pd-catalyzed reactions and synthetic work aimed at the total synthesis of guanacastepene A.

Andy's research at UMN will be in the general area of organic synthesis and enantioselective catalysis. More specifically, early projects will focus on stereoselective rearrangements and oxidations. Other research interests include continuing to expand the scope of olefin metathesis to more challenging and less explored substrates as well as exploring ability of soluble polymers to serve as supports for Lewis acid and transition metal catalysts. Ultimately, the goal of this work will be the total synthesis of structurally and biologically interesting natural products, and analogs thereof.



## 2007 Alumni Greats

**Robert P. Hammer** (Chem Ph.D. '90), a William A. Pryor Professor of Chemistry at Louisiana State University, has been named by Scientific American magazine as a research leader within the 2006 Scientific American 50, the magazine's prestigious annual list recognizing outstanding acts of leadership in science and technology from the past year. The Scientific American 50 appeared in the magazine's December 2006 issue. Hammer made the list because of his research over the last year in the basic science of Alzheimer's Disease published recently in the Journal of the American Chemical Society.



**John Franz** (Chem Ph.D. '55) recently was named a 2007 inductee of the National Inventors Hall of Fame for his discovery of the non-toxic popular weed killer Roundup®. He was honored at a special ceremony in May. Every year, the National Inventors Hall of Fame honors those whose work has changed society and improved the way we live.



Alumni: please send all your news to  
[schoenholz@chem.umn.edu](mailto:schoenholz@chem.umn.edu)

### ChemNews

Spring 2008

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## UMN Chemistry Department Makes Top Five in Country

According to the latest annual report on the number of graduates from academic departments with American Chemical Society-approved undergraduate programs, (*C&E News*, 8/20/07) the University of Minnesota ranks second after the University of California San Diego in production of Chemistry graduates (B.S., M.S., and Ph.D. combined). ACS's Big Producers Of Chemistry Graduates are

UC San Diego

UMN, Twin Cities

UNC Chapel Hill

U Illinois Urbana-Champaign

U Michigan Ann Arbor

## Professor Abul Hussam of George Mason University in Fairfax, VA has won the 2007 Grainger Challenge Prize Gold Award

from the National Academy of Engineering. Dr. Hussam was a postdoctoral associate in Professor Carr's research group at the U of M from January 1983 to August 1985, and receives the award of \$1 million for his SONO filter, a household water treatment system. At right, H.E. Shamsher of the Bangladeshi Embassy honors Dr. Hussam for his contribution at a reception on the occasion of Bangladesh's independence. For more about this award and Dr. Hussam's work, see [http://pubs.acs.org/subscribe/journals/esthag-w/2007/mar/tech/rc\\_hussam.html](http://pubs.acs.org/subscribe/journals/esthag-w/2007/mar/tech/rc_hussam.html)



Join us for a themed dinner, **Kitchen Chemistry** at the Campus Club in Coffman Union on Thursday, February 29! There will be demonstrations and a very interesting menu! Details will be available on the department website in January.

**Thanks to Sigma-Aldrich** for inviting the department to participate in its giveaway program. Several faculty members were given some very valuable chemicals and laboratory items.

## Wayne Gladfelter Named Interim IT Associate Dean for Academic Affairs

Institute of Technology Dean Steven L. Crouch has appointed long-time University of Minnesota chemistry professor Wayne Gladfelter as the college's interim associate dean for academic affairs. The half-time appointment is effective immediately and runs through June 30, 2008.

Among his many duties as interim associate dean for academic affairs, Gladfelter's responsibilities will include overseeing the processes for faculty promotion and tenure, faculty sabbatical and semester leaves, and faculty honors and awards.

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## Paul Strykowski Appointed Institute of Technology Associate Dean for Undergraduate Programs

Paul Strykowski has been named as the Institute of Technology's associate dean for undergraduate programs. This half-time appointment became effective July 1, 2007, when Strykowski started splitting his time between his new duties as associate dean and as a faculty member in the University's Department of Mechanical Engineering.

Strykowski will be responsible for devising and implementing a reorganization of the existing Institute of Technology student affairs operations during the 2007-08 school year. This will include revamping the advising system for lower division students and hiring a full-time assistant dean for student services.

## 2007 IT Graduation and Convocation Led by Chemistry Faculty

Two Chemistry faculty were honored by representing the University of Minnesota as Mace Bearers. Professor Wayland Noland, recipient of the 2006 Charles E. Bowers Faculty Teaching Award, led degree candidates to the spring 2007 IT Commencement ceremony. Professor Gary Gray, the 2000 recipient of the Mr. and Mrs. George W. Taylor Distinguished



Teaching Professorship, headed the academic procession from Coffman Union to Northrup Auditorium for the fall 2007 New Student Convocation.

The word "mace" is from Middle English and was originally used to refer to the implement for breaking armor during the Middle Ages. Today its use is more peaceful, for it now is a staff born by, carried before, or placed near a dignitary as an insignia of dignity and authority. First designed in 1961 from the inauguration of President O. Meredith Wilson, the original mace is made of aluminum and topped by a crystal ball, which symbolizes the illuminating quality and the clarity of thinking that characterizes education. The crystal ball is topped by a star representing Minnesota, the North Star State. The staff, weighing forty pounds, is carried by the most senior professor of the college present at a ceremony.

## GRADUATE AWARDS

### 2007 Graduate Research Symposium Travel Award

One of the chemistry department's academic highlights of the year is the annual Graduate Student Research Symposium. At our sixth symposium on May 15, forty-four third-year Ph.D. students presented the fruits of their research to peers, faculty, and alumni. Their talks showcased a cross-section of cutting-edge research in our department. This event continues to be a catalyst for starting new collaborations among



*Brook Carlson (Zhu group) discusses her research*

graduate students and research groups. Alumni and faculty judges provided feedback and selected the best presentation in each of four parallel sessions. This year, the distinguished alumni judges were Joseph F. Dooley (Chairman and CEO of TriMark Publications), Robert P. Hammer (William A. Pryor Professor of Chemistry at Louisiana State University), Lester C. Krogh (retired Senior Vice President of Research & Development at 3M Company), and Gilbert Walker (Canada Research Chair Professor at the University of Toronto). The overall quality of the presentations was very high, making the judges' job a difficult one. At the end of the day, four well-deserving students were each presented with a \$750 travel award: **Fan Li, Rongxiao Sa, Scott Thorgaard, and Dong Wang.** They and the other presenters have set high standards for our future symposia. Congratulations to all.



*Professor Marc Hillmyer advises above, while Chemistry Department staff Nancy Hagberg and Lynne Johnsrud keep things running smoothly*

### Nate Schultz Receives 2007 Graduate School Best Dissertation Award

Winner of the University of Minnesota Graduate School's "Best Dissertation Award" in the Physical Sciences and Engineering, Nate recently completed his Ph.D. carrying out research under the direction of Don Truhlar. He now works in the 3M Corporate Research Laboratory.

### 2006-2007 Graduate School Doctoral Dissertation Fellowship

**Kari McGee**

### 2007 Robert L. Ferm Outstanding Graduate Teaching Assistant Award

**Kelly Anderson (Outreach)**  
**Susanna Emond (for Chem. 2311)**  
**Anne Mohns (for Chem. 1022)**  
**Jason Peterson (for Chem. 1021)**

### 3M Science and Technology Fellowship

**Adam Wohl**  
**Melissa Fierke (2006)**

### MNACS Travel Grant

**Christofer Whiting**

### 2007 Graduate and Professional Student Assembly Travel Grant

**Sara Isley**

### 2007-2009 Biomedical Informatics and Computational Biology Fellowship

**George Giambasu**

### Department of Defense/American Society for Engineering Education SMART Scholarship

**Kelly Kyro**

### Department of Energy Graduate Research Environmental Award

**Mari Titcombe**

## IGERT Fellowship

Mari Titcombe

## Graduate School Fellowship

Nina Barnett

Department of Chemistry  
Graduate Fellowship

Sarah Page

Vietnam Education  
Foundation Fellowship

Anh Vu

Graham N. Gleysteen  
Fellowship in Chemistry

Aalo Gupta (2006)

Erin Arndt (2006)

Ashley Jay (2006)

Lester C. and Joan M. Krogh  
Endowed Fellowship

Craig Bishop

Amy McKeehan

Lindsay Hinkle

Eric Olson

Daniel Sadowsky

Eric Smolensky

Wayland E. Noland Fellowship  
in Organic Chemistry

Susan Brown

Melissa Jones

Susanna Emond (2006)

John Overend  
Memorial Fellowship

Nathan Burrows

Hugh Heldenbrand

Daniel O'Brien

John Wertz  
Fellowship in Chemistry

Hannah Leverentz

UNDERGRADUATE AWARDS**Chemistry Undergraduate Katie Lee Earns  
Rhodes Scholarship**

The Rhodes Scholarships, the oldest international fellowships, were initiated after the death of Cecil Rhodes in 1902, and bring outstanding students from many countries around the world to the University of Oxford. The first American Scholars were elected in 1904. Katie's citation notes that "a Goldwater Scholar, she entered the University at 15, and has done research on the human papilloma virus at Harvard Medical School. Katie is also an accomplished violinist and serves as concertmaster of the University's symphony orchestra."

**2007 Department of Chemistry  
Fellowships and Prizes**

## SENIOR AWARDS

Peteris Auzins  
Memorial Scholarship

Rachel LaFond and Han Na Park

David A. and  
Merece H. Johnson  
ScholarshipEman Haidari, David Heppner,  
Leslie O'Leary, and Sarah PageKenneth E. and  
Marion S. Owens  
Scholarship in Chemistry

Katie Lee

## JUNIOR AWARDS

Robert C. Brasted  
Memorial Fellowship

Alexander Wagner

Lloyd W. Goerke  
Scholarships

Derek Straka

M. Cannon Sneed  
Scholarship

Maris Hovlid

George T. Walker  
ScholarshipMichael DeMeuse and  
Kyle Dullinger

## SOPHOMORE AWARDS

Thomas DuBruil  
Memorial Award

Martin Donakowski

## GENERAL AWARDS

J. Lewis Maynard  
Memorial Prize in Advanced  
Inorganic Chemistry

David Heppner

CRC Freshman Chemistry  
Achievement Award

Taylor Beck

## Merck Index Award

Brian Arnold and  
Alexander WagnerUndergraduate Award in  
Analytical Chemistry

Sara Olson

Undergraduate Award in  
Environmental Chemistry

Sarah Page

**POST-DOCTORAL AWARDS 2007**

## •German Academic Exchange Service Fellowship

Stefan Huber (Cramer, Tolman)

## •U.S. Pharmacopeia Fellowship

Xiaoping Li (Carr)

# Many Thanks to our Donors in 2006

**Individual support** from alumni and friends is crucial to our department. Thanks to your generosity, we can offer fellowships and scholarships to our outstanding students, retain our best faculty, and implement projects to improve our facilities. The **Chemistry Special Projects Fund** is the department's main discretionary fund, which supports student fellowships and awards as well as the bulk of the other activities mentioned in this newsletter. With gratitude, we acknowledge our 2006-2007 donors.

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Dr Richard J Sundberg  
Mr Dale G Swan  
Dr April J Swanson  
Mr Robert F Szalapski  
Fasil A Tadesse  
Dr Laychoo Tan  
Dr Paul E Tavernier  
Texas Instruments Fdn  
Mr Brian R Thoreen  
Dr James R Throckmorton  
Mr Steven J Tinker

Dr Wade J Tornquist  
Mr Charles A Triplett  
Mr Edward T Ulrich  
Susanne M Urban  
Dr Rebecca A Urbanek  
Mr Loc X Van  
Dr Gregg A Vandesteeg  
Mr Richard E Volkmann  
Dr James R Vyvyan  
Dr James J Wade  
Dr Terence C Wagenknecht  
Ms Karen L Wallace  
Dr Edward A Walters  
Dr Hsin-Fu Wang  
Dr Joseph T Warden Jr  
Waters Corp  
Dr Mark W Watson  
Dr A Fran Watson  
Mr Edward O Welke  
Mrs Florence C Wertz  
Mr John A Wertz  
Dr Edward L Wheeler  
Mr Stephen T Wild  
Dr Larry R Wilson  
Ms Jill M Wirth  
Ms Dawn M Witherill  
Mr Wayne C Wolsey  
Dr Sharon E Worthington  
Dr Ellen L Wu  
Ms Eva C Young  
Mr Thomas K Yue  
Dr Lee R Zehner  
Dr Hongyu Zhao  
Mr Mohammad S Zia-Ebrahimi



## **Dr. Peter Chen, ETH (Swiss Federal Institute of Technology), is Fall 2006 Gassman Lecturer**

*Gassman Lecturer Peter Chen relaxed after his seminar with faculty and visitors. From left to right: David Blank, Gerda Gassman, Peter Chen, Christy Haynes, and Bill Tolman.*



**Don  
Truhlar**

## **Regents Professorship**

The Regents Professor position was established in 1965 by the Board of Regents to recognize the national and international prominence of faculty members. It serves as the highest recognition for faculty who have made unique contributions to the quality of the University of Minnesota through exceptional accomplishments in teaching, research and scholarship or creative work, and contributions to the public good.

A citation from the nomination letter states, "Don Truhlar has served the University with distinction for over 35 years, during which time he has established an unsurpassed record in research, teaching, and service. His stature as a scholar is immense, broad-based, and international; he is among the most brilliant and distinguished physical scientists of his generation. He has advised and trained huge numbers of students in the area of computational chemistry, many of whom many have gone on to build their own distinguished careers. Finally, he has generously given his time (and applied his formidable organizational abilities) to the betterment of his discipline and the University of Minnesota. Professor Truhlar epitomizes, in my view, a Regents Professor: a brilliant and productive scholar, a dedicated and sensitive mentor and advisor, and an untiring worker on behalf of the University."

Only two other chemistry professors have been recognized with this distinct honor: Bryce Crawford, Jr., (1982) and Paul G. Gassman (1988).

## **Wayne Gladfelter and Bill Tolman**

### **American Association for the Advancement of Science Fellow**



Election as a Fellow of AAAS is an honor bestowed upon members by their peers. Fellows are recognized for meritorious efforts to advance science or its applications. Newly elected Fellows (2006) were recognized for their contributions to science and technology at the Fellows Forum held on 17 February 2007 during the AAAS Annual Meeting in San Francisco. The new Fellows received a certificate and a blue and gold rosette as a symbol of their distinguished accomplishments.

Other fellows include Professors Noland (1987), Truhlar (1994), and Que (2001).

## **Christy Haynes**

### **McKnight Land- Grant Professorship**

The major purpose of the McKnight Land-Grant Professorship program is to nurture the careers of the University of Minnesota's most promising junior faculty members in order to strengthen the faculty for the future. The program is designed to advance the careers of assistant professors who are at the beginning stages of their professional careers, and who have the potential to make significant contributions to their scholarly fields. The program is also



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*continued on page 14*

Website:

[www.chem.umn.edu/microscopycamp](http://www.chem.umn.edu/microscopycamp)



UNIVERSITY OF MINNESOTA  
Driven to Discover<sup>SM</sup>

# Microscop

## Search Results Microscopy Camp

- What are crystals made of?
- What's the difference between salt and sugar crystals?
- Can we see atoms?
- What is the current model of atomic structure?
- What equipment is used to image objects at atomic resolution?
- How can we teach students about the particulate nature of matter?
- How small is nano?
- How is nanotechnology important to me and people close to me?



**Profs. Penn** (Chemistry) and **Flynn** (Science Education) have developed and implemented Microscopy Camp, and the above is just a small sampling of the questions they address. Microscopy Camp is designed to introduce and reinforce concepts of the atomic structure of solid crystals to middle school-age students. To date, twenty students have attended Microscopy Camp, which was first held over two days at the University of Minnesota in August of 2005 and then 2006 and funded by Prof. Penn's NSF CAREER award. Campers synthesized their own magnetite ( $\text{Fe}_3\text{O}_4$ ) nanoparticles; characterized their particles using visual inspection, hand-held magnifiers, light microscopes, and hand-held permanent magnets; and participated in the characterization of their particles using scanning electron microscopy (SEM) and high-resolution transmission electron microscopy (HRTEM). For most students in this age group, this type of experience provides the first opportunity



directly contradicts real world experience with objects like the bricks used to construct buildings and houses. Pre-camp and post-camp assessments were conducted, and qualitative results demonstrate improved post-camp understanding in 80% of the participants (results appeared in *Journal of Chemical Education* in June of 2007).

to directly observe the atomic structure of solid crystalline materials.

An interesting and common misconception in this age group is the idea that larger crystals have larger atoms than do smaller crystals. This idea





# Microscopy Camp

Student teachers have been integral to the design and implementation of Microscopy Camp, including two chemistry majors (David Quosig in 2006 and Spencer Ladd in 2001-2002). In addition, Joe Franek (Lecture Demonstration Director) has designed and implemented a dazzling array of demonstrations, including explosions and syntheses (such as goo and ferrofluid). A particularly wonderful example was his demonstration of Brownian Motion using cigarette smoke for Microscopy Camp 2007 (available for viewing at youtube.com).

Microscopy Camp 2007 (July 30-August 3, 2007) was expanded, and funded



through the Department of Education, to serve middle school and high school science teachers. Nineteen teachers from around Minnesota and Wisconsin attended MC 2007, including Per Lee, who took Prof. Penn's Chemistry 1022 (General Chemistry II) course in 2001!



**Microscopy Camp Cheer**  
 (written by three campers from MC 2005)

We exploded things and made some goo,  
 We had fun, how 'bout you?  
 We had pizza and subs for lunch,  
 Chips, drinks, and yummy things to  
 munch!  
 We mixed and boiled and bubbled and  
 brewed,  
 We made fire, and it turned blue!  
 We looked at bugs under a microscope,  
 We learned new things and made stuff  
 too!  
 We looked at a microscope that magnifies  
 a million,  
 We had fun, **TIMES A ZILLION!**

...It was great to return to Smith Hall. Every time I go by the building it brings back good memories, and maybe a few bad ones. It was also great to see some familiar faces in the building such as yourself and other faculty. It was also neat to see that there had been some changes to the building such as smith 100. Microscopy camp was a great experience. It was the last class I needed to complete my masters in education and I can't think of another class that I would have gotten more out of. Much of the content was new to me or at least presented in a new way. Something that I thought was great was that all of the activities were done in a way that they could be directly used in our own classrooms. It was very cool to see and use the different electron microscopes. I will definitely be sharing the images we captured with my students and colleagues. I had such a good time with Microscopy camp that I hope to return in the future as a facilitator so I can take what I learned and pass it on to new students.

Per Lee, 1022 student, 2001

intended to foster an esprit de corps among these future faculty leaders, and to help build a sense of loyalty to the institution.

Dr Haynes is at the very early stages of setting up her independent research program. Nevertheless, her exceptional broad training, which combines laser spectroscopy and nanomaterials characterization (the subject of her graduate research) with electrochemistry and neurobiology (her post-doctoral work), has enabled her to launch a unique research program that addresses scientific questions at the interface of neurobiology, materials science, and chemistry. Her research has brought innovative, new ideas to the area of bioanalytical chemistry, which is a developing strength at the University of Minnesota.”

Professors Doreen Leopold (1987), Stephen Kass (1988), Ken Leopold (1989), Jeff Roberts (1991), Bill Tolman (1992), Christopher Cramer (1994), Ilja Siepmann (1996), Andreas Stein (1997), Marc Hillmyer (2000), Kris McNeill (2004), and Andy Taton (2005) have also received the McKnight Land-Grant Professorship.

## Tom Hoyer

### **Horace T. Morse/University of Minnesota Alumni Award for Outstanding Contributions to Undergraduate Education**



*Tom Hoyer, back row center, with other Morse and postbaccalaureate awardees (left to right seated) Joel Samaha, John Day, Praveen Aggarwal, Paula O'Loughlin, Ned Mohan, Maria Damon, and Patricia James and (standing) Bruce Wollenberg, Ruth Lundquist, Jay Bell, and Tom Molitor*

Each year since 1965, the University of Minnesota has recognized a select group of faculty members for their outstanding contributions to undergraduate education. This honor is awarded to exceptional candidates nominated by colleges in their quest to identify excellence in undergraduate education. In addition to honoring individual faculty members, the award contributes to the improvement of undergraduate education at the University by publicizing their work to serve as a resource for the whole faculty. The award, named for a former dean of General College, is made possible through generous support of the University of Minnesota Alumni Association and the Office of the Senior Vice President for Academic Affairs and Provost.

A former student of Professor Hoyer writes, “I feel very fortunate that Professor Hoyer works so hard to make unique opportunities available for undergraduates. Because of him, I have been able to test the limits of my capabilities and feel confident in my future as a chemist who can make a difference. His genuine concern, support, and encouragement, especially through most difficult times, set him apart from other professors.”

## Attention Alumni

Send us your update to either:  
[www.chem.umn.edu/alumni/contact.html](http://www.chem.umn.edu/alumni/contact.html)  
or  
[alumni@chem.umn.edu](mailto:alumni@chem.umn.edu)

Let us know what you think.

We want this publication to reflect your interests. Send comments to:

ChemNews  
Department of Chemistry  
207 Pleasant Street S.E.  
Minneapolis, MN 55455  
or  
[chemnews@chem.umn.edu](mailto:chemnews@chem.umn.edu)

Seven other chemistry professors have received this award: Robert Brasted [deceased] (1970), Lou Pignolet (1990), Larry Miller [retired] (1993), Gary Gray (1996), Kent Mann (2003), Ken Leopold (2005), and Mark Distefano (2006).



## Marc Hillmyer

### George W. Taylor/ IT Alumni Society Award for Research

Established in 1982, the Taylor Award for Distinguished Research recognizes younger faculty

members who have shown outstanding ability in research.

One supporting letter states, "Marc has established himself as a rising star in the field of macromolecular science. What separates Marc from his peers is his unique ability to combine synthetic chemistry with sound physical insight on problems that are both fundamentally significant and technologically relevant. Based on his past performance, I believe his trajectory is unmistakable, and it would be fitting to honor him at this time for his impressive achievements."

Professor Hillmyer joins Bill Tolman (1998), Chris Cramer (1999), and Tim Lodge (1993) in receiving this distinguished award.



## Larry Que

### 2008 ACS Alfred Bader Award in Bioinorganic or Bioorganic Chemistry

This national American Chemical Society Award recognizes outstanding contributions to bioorganic or bioinorganic chemistry. The award consists of \$5,000 and a certificate. Professor Que will be invited to contribute an article based on the award address to *Aldrichimica Acta*.

Professor Larry Que's research over the past several decades has changed the way we think about the chemistry of non-heme iron proteins and complexes, and has placed him amongst the most prolific and important practitioners of bioinorganic chemistry in the world.

Professor Que has played a pioneering role in understanding the function that nonheme iron centers play in dioxygen activation in biology. Using a truly multidisciplinary approach, he successfully combined biochemical/biophysical studies of the metalloproteins themselves and synthetic approaches to develop structural and functional models for these systems. This synergistic process allowed his group to develop the most complete picture possible for the metal coordination site and its role in catalysis. Mononuclear enzymes of interest catalyze a diverse array of metabolically important transformations that include hydroxylation of aliphatic and aromatic C-H bonds, heterocyclic ring formation, arene cis-dihydroxylation, and oxidative ring cleavage. Many of these enzymes utilize a common 2-His-1-carboxylate facial triad motif first recognized by Que as a common platform for dioxygen activation. Enzymes of interest also share a common diiron site to activate dioxygen and carry out alkane hydroxylation, fatty acid dehydrogenation, and arene hydroxylation.

Recent recipients of this distinguished award include Peter G. Schultz (2001), Ronald Breslow (2002), Christopher T. Walsh (2003), Stephen J. Lippard (2004), Alan R. Fersht (2005), F. Ann Walker (2006), and Eckard Munck (2007).



Larry Que is toasted by Chair Jeff Roberts at the Campus Club

## 2006 Civil Service Award Winners

Frank Dandl  
Sheryl Frankel  
Michael Kurth  
Renae Wasylishin

## New Hires in Chemistry

**Ben Geisbauer** has been hired to take over Frank Dandl's position. Ben was born in St. Paul and grew up in Forest Lake, MN where he graduated from high school and where he currently resides. Ben attended and graduated from Century College in White Bear Lake, MN with a degree in automotive service. In his spare time, Ben likes to fish, hunt small game and bow hunt for deer.

### **Roxanne M. Horky**

replaces Anne Mockovak as Chief Financial Officer. Roxanne was a fiscal officer in the S.O.U.P. budget office, an administrative cluster for the Departments of Surgery, Orthopaedic Surgery, Urologic Surgery, and Physical Medicine and Rehabilitation. She started her Chemistry appointment on August 17, 2006.

**Sophia Herrera** has also joined the Chemistry Accounting Office as our accounts payable coordinator. Sophia came to us with several years of University experience and will be a terrific addition to our team.

**WELCOME TO THE  
CHEMISTRY DEPARTMENT!**

**Dale Randall** has once again received a Sigma Aldrich Professional Development Fund Award for travel to the 34th Annual Conference and Trade Show. Congratulations, Dale.

## Two Long-Time Chemistry Staff Members Ring Retirement Bells!

**Handiest Man  
Frank Dandl**

**Lab Director  
Barb Edgar**

**Frank Dandl** retired after thirty-one years as our "M&O Mechanic." His retirement party was held in Smith Hall 117/119 on Frank's last day on the job, June 1, 2007.



After over twenty years of service to the Department of Chemistry, as a lecturer and as Director of General Chemistry, **Barb Edgar** retired on May 18, 2007. A reception in her honor was held in 117/119 Smith Hall.



*Flurnia Hadley-Davis and Kathy Ross enjoy the atmosphere and the food! at Frank's send off*



*Mailroom honcho Vic Munsch and replacement Ben Geisbauer give Frank a big goodbye*

# Fall Graduate Welcome Party a Hit - Again!

Make Your Donation  
to the Chemistry Department's  
**Special Projects Fund**

by enclosing your gift in the envelope  
provided in the back of this newsletter.  
Help support our faculty and students.



*Thanks to Chuck Tomlinson for providing the entertainment!*



# Chemistry Degrees Granted

July 1, 2006 to June 30, 2007

Ph.D. Degrees	Advisor	Thesis Title
Ziyad F Al-rashid	Hoye	<i>Structure Determination and Total Synthesis of Rasfonin.</i>
Amy J Anschutz	Penn	<i>Reactivity of Iron Oxyhydroxide Nanoparticles: Effects of Physical Variables.</i>
Anne L Boreen	McNeill	<i>Enhanced Photolysis in Natural Waters: Naturally Occurring Sensitizers, Substrates, and Applications to the Fate of Aquatic Pollutants.</i>
Carolyn S Brauer	Leopold, K	<i>Microsolvation of Reactive Systems in the Gas Phase via Fourier Transform Microwave Spectroscopy.</i>
Michael William Burand	Mann	<i>Synthesis and Characterization of Oligothiophene-Based Compounds for Use as Semiconducting Materials in Thin-Film Transistors.</i>
Jason Robert Burney	Mann	<i>Synthesis and Characterization of Platinum (II) Complexes for Use as Environmental Sensors.</i>
Yun Chen	Arriaga	<i>Determination of Doxorubicin Content of Individual Endocytic Organelles by Capillary Electrophoresis with Laser-Induced Fluorescence Detection.</i>
Benjamin Patrick Duckworth	Distefano	<i>Site-selection Modification of Proteins Using Protein Farnesyltransferase.</i>
Gregory John Dutton	Zhu	<i>Electronic Structure and Ultrafast Dynamics in Molecular Films on Metal Surfaces.</i>
Becky L Eggimann	Siepmann, Veglia	<i>Monte Carlo Simulations for NMR-based Protein Structure Determination, Aqueous Interfacial Properties, and Pressure-Volume Curves.</i>
Benjamin Andrei Ellingson	Truhlar	<i>Quantum Mechanical Methods for Calculating the Thermodynamics of Molecules with Hindered Rotations and the Rates of Chemical Reactions.</i>
Nicholas S Ergang	Stein	<i>Design and Fabrication of Nanostructured Materials for Power Generation and Nanocomposites.</i>
Angela D Follett	McNeill	<i>Explorations into the Mechanism and Kinetics of the Reduction of Trichloroethylene Using Model Complexes of Cobalamin and Zero-Valent Iron.</i>
Joseph M Fritsch	McNeill	<i>Studies on the Catalytic Reductive Dehalogenation of Chlorinated Ethylenes and the Preparation of Tetradentate Beta-Diketiminato Complexes.</i>
Aimee R Herdt	Taton	<i>Engineering Biomolecules and Nanostructures for Bioconjugate Chemistry.</i>
Shengxiang Ji	Hoye, Macosko	N.A.
James Edward Kabrhel	Hoye	<i>Part I: Is a Cope Rearrangement Viable as the Key Feature in the Biosynthesis of (+)-Ottelione A? Part II: The No-D Study of the n-BuLi Oxidation of 1,5-Cyclooctadiene.</i>
Casey P Kelly	Cramer, Truhlar	<i>Implicit Solvation Models for Air-Water Interfaces and Aqueous and Nonaqueous Solution.</i>
Byeong-Su Kim	Taton	<i>Encapsulation of Nanoparticles in Block Copolymer Micelles and Application in Biotechnology.</i>
Castro Sam Laicer	Taton	<i>Controlling Self-Assembly and Anisotropy of Block Copolymer Materials with Nanorods.</i>
Yongfeng Li	Forsyth	<i>Synthetic Studies Towards the C1-C20 Bis-spiroketal Domain of Azaspiracid.</i>
Zhibo Li	Lodge, Hillmyer	<i>Multicompartment Micelles from ABC Miktoarm Star Terpolymers in Water.</i>
Hao Luo	Carr	<i>A Silica-Based Hydrophobic Cation Exchange Phase for Water Soluble Pharmaceuticals and Bioactive Analytes.</i>
Huiming Mao	Hillmyer	<i>Nanoporous Polymers with Functionalized 1-D and 3-D Channels from Ordered Block Copolymer Templates.</i>
Matthew Joseph McGrath	Siepmann	<i>Monte Carlo Simulations of Hydrogen Bonding Fluids.</i>
Danni Li Meany	Arriaga	<i>Mitochondrial Superoxide Production and its Oxidative Damage to Proteins.</i>
Randy A Mroze	Taton	<i>Preferential Nucleation and Alignment of Polymer Mesophases by Carbon Nanotubes.</i>

# Chemistry Degrees Granted

July 1, 2006 to June 30, 2007

Ph.D. Degrees	Advisor	Thesis Title
Timothy J Murray	Forsyth	<i>A Total Synthesis of Gex1a.</i>
Kwangho Nam	Gao, York	<i>Quantum Mechanical/Molecular Mechanical Studies of Haloalkane Dehalogenase and Hairpin Ribozyme.</i>
Son Truong Nguyen	Forsyth	<i>Synthesis of the ABCD and FGHI Domains of Azaspiracid.</i>
Adam Peter Schellinger	Carr	<i>Improving the Speed, Transferability and Optimization of Gradient Elution Reversed-Phase Liquid Chromatography.</i>
Kathleen M Schreck	Hillmyer	<i>Renewable, Degradable Polymers for Polylactide Toughening.</i>
Nathan Eugene Schultz	Truhlar	<i>Computational Nanoscience.</i>
Li Sun	Siepmann	<i>Monte Carlo Simulations for Chromatographic Systems.</i>
Victor J Sussman	Ellis	<i>Studies on the Chemistry of Low-Valent Polyarenometalates of Niobium and Tantalum.</i>
Timothy Michael Trygstad	Forsyth	<i>Versatile Synthesis of the C3-C14 Domain of 7-Deoxyokadaic Acid and Strategic Analogues.</i>
My-Nuong Thi Vo	Musier-Forsyth	<i>Mechanistic Studies of the Nucleic Acid Chaperone Activity of HIV-1 Nucleocapsid Protein.</i>
Bo Wang	Forsyth	<i>Chemistry and Biology of Phorboxazoles.</i>
Ce Wang	Forsyth	<i>Synthesis and Methodology Development Towards Natural Products: Okadaic Acid and Spirastrellolide A.</i>
Xiaoli Wang	Carr, Mann	<i>Part I. Fundamental and Applied Studies of Chromatographic Resolving Power for Use in Proteomic Analysis. Part II. Transition Metal Based Chiral Stationary Phases for Enantiomeric Separations.</i>
Jianyan Xu	Forsyth	<i>Progress Towards the Total Synthesis of Azaspiracids.</i>
Lu Ying	Forsyth	<i>Synthesis of Phorboxazole A Analogs Via Quick Structural Diversification.</i>
John Thomas York	Tolman	<i>Application of N-Donor Ligated Copper Complexes in Dioxygen Activation and the Synthesis of Copper-Sulfur Clusters Relevant to Biology.</i>

## Master's Degrees

## Advisor

## Thesis Title

Sarah A Barfknecht	Forsyth	<i>AuCl Catalyzed Spiroketalization in the Synthesis of the C16-C27 Central Core of Okadaic Acid.</i>
David Degrio	Que	N.A.
Brendan Edward Gordon	Mann	
Ayako Hosokawa	Distefano	<i>Kinetic Studies of Alkyne-Containing Analogues of GPP and FPP Using a Continuous Fluorescence Assay and Mechanistic Studies of Protein Farnesyl Transferase.</i>
Shuang Liang	Forsyth	<i>Synthesis of the C21-C40 Domain of Azaspiracid-3.</i>
Elizabeth C Lugert	Buhlmann	<i>Perfluoropolymers: Plasticization for Application in Ion-Selective Electrodes.</i>
Emily Skowronek Resar	Bowser	<i>Plan B</i>
Nikolay Viktorovich Voskoboev	Musier-Forsyth	<i>Exploring the Hydrolytic Editing Activity, Substrate Specificity, and Function of the Enterococcus Faecalis YbaK Protein.</i>
Leslie Jaye-Anne Warner	Buhlmann	<i>Effect of Electrically Neutral Compounds on the Response of Fluorous Membrane-based Ion Selective Electrodes.</i>
Nicholas David Zunker	Forsyth	<i>Synthesis of the C31-C46 Domain of Phorboxazole Analogs.</i>

## Bachelor's Degrees and Home Town

Daniel Yeboah Achina	Accra, Ghana	Rachel Jean Lafond	Walker, MN
Joshua William Allen	White Bear Lake, MN	Jeffrey Michael Lanners	New Richmond, WI
Jack Everett Anderson	Osseo, MN	Matthew James Lindquist	New Prague, MN
Anay Bedi	Plymouth, MN	Donald Fred Machovsky III	Brooklyn Park, MN
Trevor Allen Bieber	Golden Valley, MN	Mariam Akbar Malik	North Oaks, MN
Nathan Thomas Bradbury	Wilston, ND	Matthew Emile Marquis	Esko, MN
Eric Edward Buck	Lakeville, MN	Tate Matthew Mathiason	Roseville, MN
Kimberly Marion Burke	Mounds View, MN	Elliot James McSherry	Woodbury, MN
Jamie Lynn Cameron	Wayzata, MN	Airee V Mobley	Kansas City, MO
Darrin L Carlson	Minneapolis, MN	Steven Ray Neumann	Caledonia, MN
Geoffrey Scott Carlson	St. Cloud, MN	Son T Nguyen	Vietnam
Jennifer Ann Carlson	Oak Grove, MN	Tho H Nguyen	St. Cloud, MN
Bunkosal Chhun	Richfield, MN	James H Nik-khah	Kansas City, MO
Aaron Allen Christoffersen	Woodbury, MN	Sara Marie Olson	Plymouth, MN
Stephen Corey Codoluto	Inver Grove Heights, MN	Sarah E Page	Golden Valley, MN
Carin Nichole Curtis	Champlin, MN	Han na Park	Roseville, MN
James H Dahlstrom	Blaine, MN	Kihong D Park	Wayzata, MN
Trinh T Dang	Vietnam	Christopher Paskach	Plymouth, MN
Allison Marie Darsow	White Bear Lake, MN	Yogesh A Patel	Brooklyn Park, MN
Sarah Ann Delo	Elkhorn, WI	Joel T Pehoski	Maplewood, MN
Joshua T Dickman	Hudson, WI	Mike J Perbix	St. Paul, MN
Jay William Draves	De Pere, WI	David Alan Quosig	Milwaukee, WI
Alicia Ann Engbrecht	Eden Prairie, MN	Galen Edward Rahmlow	Kansas City, MO
Jill Nichole Evers	Oakdale, MN	April A Rasdal	Sioux Falls, SD
Kristin Marie Ficek	Brookfield, WI	Sanjeeva Ratnayake	Columbo, Sri Lanka
Lisa Anne Garton	Eagan MN	Matthew Steven Rauschke	Blaine, MN
Simon J Gruber	St. Louis Park, MN	Molly E Reardon	Robbinsdale, MN
Eman Sattaree Haidari	Eden Prairie, MN	Christopher J Reindl	Sun Prairie, WI
Heidi Jane Hammerschmidt	Eagan, MN	Christopher Rogers	Fridley, MN
Gregory M Hanggi II	Kingwood, TX	Caitlin Emily Rooney	Marine on St. Croix, MN
Ricky Hartono	Indonesia	Amanda Lea Ryczek	Portage, WI
Muqbil Omar Hashi	Eden Prairie, MN	Nicholas Enrique Sanchez	Lakeville, MN
David Earl Heppner	Chicago, IL	Monica Santos-Martinez	Plymouth, MN
Laura E Hiti	Plymouth, WI	Chad Patrick Satori	Valders, WI
Vincent Carl Holmberg	Circle Pines, MN	Zackary John Schmidt	Inver Grove Heights, MN
Nor Fariza Ismail	Malaysia	Luke Charles Schuster	Mendota Heights, MN
Keith Russell Jacobs	New Berlin, WI	Matthew Joseph Stastny	Kohler, WI
Christina M Jahnke	Pewaukee, WI	Jennifer Erin Stavseth	Cokato, MN
Philip Joseph Jarzombeck	Oregon, WI	Jonathan E Stromme	St. Cloud, MN
Emily C Jenson	Minneapolis, MN	Lidin L. Su	Brooklyn Park, MN
Jenna M Johnson	Plymouth, MN	Corrine Marie Sullivan	Woodbury, MN
Caleb William Jones	Minneapolis MN	James A Swakow	Des Plaines, IA
Ross Michael Jorenby	Madison, WI	Jason A Taubel	Fredericksburg, VA
Felicia Grace Kadarusman	Jakarta, Indonesia	Cassidy R Terrell	Lakeville, MN
Bria Katherine Kaiser	Delano, MN	Craig Franz Tschautscher	Carver, MN
Catherine Kallaus	Apple Valley, MN	Abraham Tsehay	Minneapolis, MN
Ashley Nicole Kleis	Hastings, MN	Kristine Nicole Vogt	Richfield, MN
Valerie Marie Kramlinger	Arden Hills, MN	Peter J Wegwerth	Byron, MN
Kristine M Kun	Apple Valley, MN	Thomas MartinWessling	Oconomowoc, WI
William Newell Kusch	Madison, WI		

# Molding Porous Nanoparticles

## Recent research from Professor Andreas Stein and his research group

Within the last few years, nanoparticles have transitioned from scientific curiosities to becoming essential components in applications such as sensing, nanoelectronics, catalysis and other uses. Their unique optical, electronic, magnetic and reactive properties compared to bulk solids rely on control over both the size of the particles in the nanometer size-regime and the particle shapes. But how can the synthetic chemist control shapes on such a small scale? Graduate student Fan Li in the Stein group recently developed a novel approach for preparing monodisperse, discrete nanoparticles with specific shapes (e.g., cubes, tetrapods, spheres). These shaped particles can be porous, thereby significantly enhancing surface areas of the particles and opening up possibilities for host-guest applications (e.g., sensors). The method is based on a combination of self-assembly and templating methods in tandem with controlled disassembly of porous solids into their structural building blocks (Figure 1).

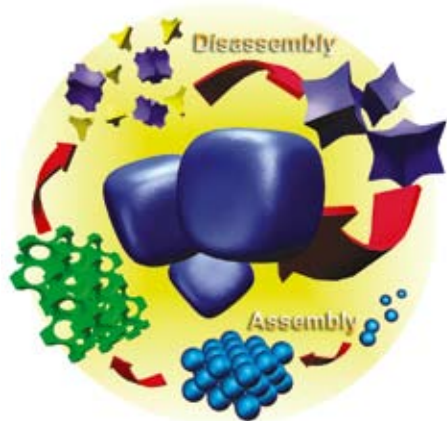


Figure 1. Porous silica nanocubes and tetrapods are produced when a bottom-up synthesis based on natural assembly/templating methods is combined with a top-down synthesis involving structural disassembly. Uniform polymer nanospheres are assembled into close packed arrays like marbles in a box. The space between spheres is filled with precursors. During heating the polymer spheres are removed and a solid spongy skeleton forms. Under the appropriate reaction conditions, the skeleton breaks down into uniform building blocks.

Shaped silica nanoparticles are prepared by controlled disassembly of a solid skeleton that is built around a scaffold of close-packed nanospheres. The skeletal structure consists of two basic units, cubes and tetrapods, which correspond to the space between the packed nanospheres and are connected like tinker-toys. Fan Li discovered that these building blocks can be disconnected and isolated under specific synthesis conditions (Figure 2). The disassembly occurs first by thinning of the necks between the two units, followed by complete disconnection of the skeleton at the narrowest connection points. Discrete nanoparticles are obtained in high yield. Their sizes are easily controlled by the diameters of the templating nanospheres. The sponge-like silica nanocubes and tetrapods can themselves be used as molds to produce similar particles made of carbon or polymers. This general method of preparing uniform porous nanoparticles with specific shapes is described in an upcoming issue of *Angewandte Chemie*, International Edition and is featured on the journal cover. ■

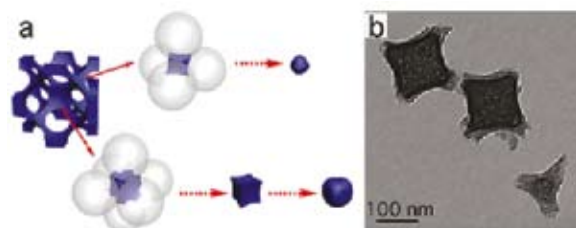
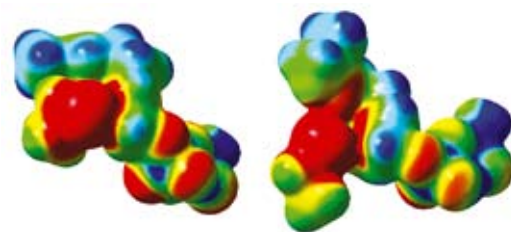


Figure 2. (a) Illustration of the disassembly of a porous skeleton structure into its building blocks. (b) Transmission electron microscopy image of carbon replicas of the porous silica cubes and tetrapods.

# Transition State Analysis of the Chemical and Enzymatic Prenylation Reactions

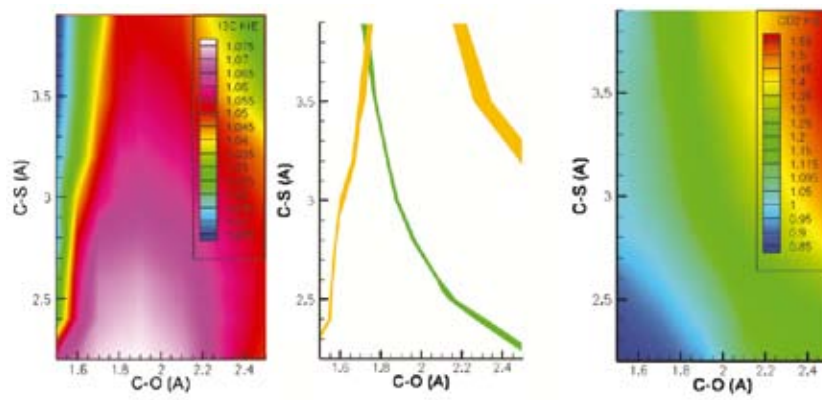
## Professor Mark Distefano and his group

Protein prenylation involves the attachment of C15 (farnesyl) or C20 (geranylgeranyl) groups to proteins and is catalyzed by a class of enzymes known as prenyltransferases. The observation that inhibition of Ras farnesylation arrests the growth of tumor cells has been the motivating factor in developing inhibitors of prenyltransferases that can serve as anticancer drugs; currently several candidates are in Phase 3 clinical trials. We are interested in using kinetic isotope effect (KIE) measurements to determine the transition state (TS) structure for the enzyme catalyzed reaction since knowledge of the TS structure may allow the selectivity and affinity of inhibitors of these enzymes to be improved. Recently, graduates students Stepan Lenevich and Ayako Hosakawa, and Postdoctoral Fellow Dr. Juhua Xu in the research group of Professor Mark Distefano measured a primary  $^{13}\text{C}$  KIE and a secondary  $^2\text{H}$  KIE via mass spectrometry. In collaboration with Professor Chris Cramer, a TS structure for the farnesyltransferase enzyme-catalyzed reaction was computed; a density functional level of electronic structure theory using the mPW1N functional in combination with the 6-31+G(d) basis set was employed for those calculations. The results indicate that the enzyme effects catalysis via an “exploded” TS structure with an extended C-S bond. This is the first example of a transition state structure obtained from an enzyme catalyzed prenylation reaction and was recently published in the Journal of the American Chemical Society (DOI: 10.1021/ja069119j)



KIE analysis of the prenylation reaction catalyzed by protein-farnesyltransferase. 3D Contour plots of KIEs versus C-O and C-S bond lengths. Left panel: Plot of calculated primary  $[1-^{13}\text{C}]$  KIE (z-axis, color contours) versus C-O (x-axis) and C-S (y-axis) bond lengths. Right panel: Plot of calculated secondary  $[1-^2\text{H}]_2$  KIE (z-axis, color contours) versus C-O (x-axis) and C-S (y-axis) bond lengths. Center panel: Superposition of calculated contours from Left and Right panels that match the experimentally determined values of the  $[1-^{13}\text{C}]$  KIE (orange) and  $[1-^2\text{H}]_2$  KIE (green). The region of intersection gives the C-O and C-S bond lengths in the TS.

Transition state structures for nonenzymatic reaction between GPP and ethane thiolate and the corresponding enzyme catalyzed reaction. TS structures were modeled in the gas phase at the mPW1N/6-31G\* level of theory. Electrostatic potentials: Left panel, nonenzymatic reaction; Right panel, enzymatic process. Red represents more negative potential (-0.15 au), blue represents less negative potential (-0.05 au) and green is intermediate (-0.10 au). The electrostatic potentials are presented mapped on the 0.005 au isodensity surface. ■

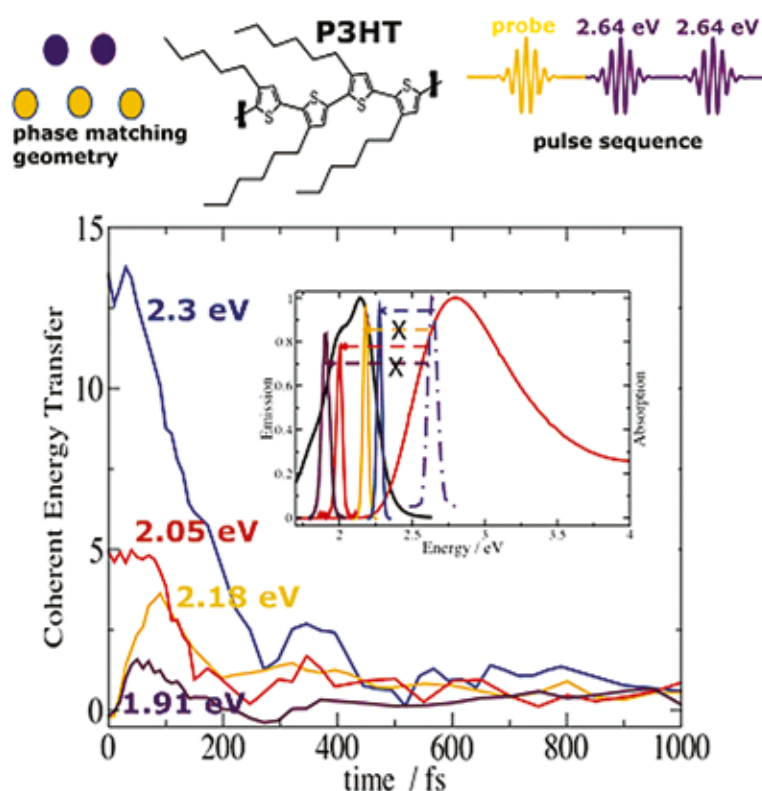


# Correlated Ultrafast Exciton Relaxation in Conducting Polymers

Professor David Blank and his group

Poly-3-hexylthiophene, or P3HT, is one of the most commonly used organic conductors in opto-electronic research. This material is often employed as both a light harvester and hole conductor in the development of new photovoltaic devices. Using ultrafast spectroscopy, graduate student Nathan Wells has been investigating the dynamics that follow light absorption in these molecules. After a photon creates a bound electron-hole pair, called an exciton, both nuclear reorganization and migration to segments of longer conjugation lengths lower the energy of the exciton. One of the interesting parts of this process is that a significant portion of the exciton cooling takes place in less than 100 femtoseconds. Using 2-color 3-photon echo spectroscopy (2C3PES), Nathan has demonstrated that transfer from the initial excitation energy is coherent and correlated to specific energies in the fluorescence band, i.e. the energy does not simply run downhill. This is shown in the graphic below, where the signals are directly related to coherent transfer of energy from the excitation at 2.64 eV to four different energies in the fluorescence band. Note that within the time resolution of the experiment ( $\sim 30$  femtoseconds), coherent transfer has already taken place at 2.30 eV and 2.05 eV, but it is initially zero and builds in over time at 2.18 eV and 1.91 eV. These measurements demonstrate that the initial rapid localization of the exciton is spectrally correlated, and cooling then continues with nuclear motions such as displaced torsions that allow the exciton to sample the rest of the fluorescence band. Understanding the electronic-nuclear coupling in these organic materials can provide a foundation for understanding how to design a better photovoltaic.

This research was supported by the University of Minnesota Initiative for Renewable Energy and the Environment (IREE) and the David and Lucile Packard Foundation. ■



# Institute of Technology Hosts Honeywell Nobel Laureate

**Dr. Roderick MacKinnon** was the featured Nobel laureate for the Honeywell-Nobel Initiative event on October 1–2 at the University of Minnesota-Twin Cities. The University of Minnesota is one of only 11 universities worldwide, and five in the United States, selected to participate in this program.



Awarded the 2003 Nobel Prize in Chemistry for his discoveries concerning the molecular mechanisms in cell membranes, MacKinnon delivered a lecture on “Electricity in Biology” at the University of Minnesota McNamara Alumni Center, Memorial Hall. The event was free and open to the public. The lecture was also webcast live. Currently at Rockefeller University, MacKinnon is the John D. Rockefeller Jr. professor in the laboratory of molecular neurobiology and biophysics and investigator of the Howard Hughes Medical Institute.

The lecture, which served as the centerpiece of his two-day visit with university students, highlighted the modern understanding of electrical systems in living organisms, specifically the electricity in living cells. MacKinnon also will explain how this topic exemplifies the strange and unexpected manner in which scientific ideas evolve.

In addition to the lecture, MacKinnon was involved in several other campus events including speaking in an undergraduate chemistry class, discussing research with graduate students and meeting with faculty, providing unique opportunities for students and faculty to interact with Nobel laureates in an intimate setting in order to gain insight into what it means to be an innovator in science.

The schedule of public events included the lecture, an interactive Honeywell Traveling Technology Experience (TTE), and a poster session for Institute of Technology graduate student research.

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