DECEMBER 2012

College of Science & Engineering
University of Minnesota

# CHEM news

DEPARTMENT OF CHEMISTRY NEWSLETTER

## Inside this issue…



# Graduate students & postdoctoral researchers lead laboratory safety efforts

*From safety-themed posters to informative safety moments before meetings and seminars, creation of a safety website, and an increased emphasis on wearing proper safety gear in laboratories, graduate students and postdoctoral researchers are taking the lead*

**Safety Starts with U**

in improving and sustaining the safety culture in the University of Minnesota College of Science & Engineering's chemistry and chemical engineering laboratories. This fall, they kicked off a new safety campaign, "Safety Starts with U!"

Through a unique partnership with the Dow Chemical Company, graduate students and postdoctoral researchers from the departments of Chemistry (CHEM) and Chemical Engineering and Materials Science (CEMS) are providing the leadership to a first-ever pilot program to improve safety awareness and practices. While the Dow Chemical Company is not providing a financial donation to the University of Minnesota for this safety initiative, it is sharing its best-in-class laboratory safety practices, examples, advice, and resources with U of M students and postdoctorates. Last spring, Dow sponsored a two-day safety training for students and faculty at its facility in Michigan, and since then, it has been providing ongoing advice to the graduate students and post doctorates.

Kathryn "Kate" McGarry, a graduate student in the Department of Chemistry and chair of the Joint Safety Team Administrative Committee, demonstrates how hoods and protective glass are important safety features that need to be used appropriately in laboratories, as is wearing personal protective equipment.

"Ensuring safe working environments in research laboratories is both a challenge as well as an

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CHEM news

DECEMBER 2012

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*Photo of Christy Haynes by Steve Niedorf*



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# Our highlights include partnerships, research, student and faculty accomplishments

Chair William Tolman

*Welcome to the fall 2012 edition of our printed newsletter. We have enhanced its appearance. We hope you enjoy reading about all of the exciting happenings that have occurred in the Department of Chemistry this past year.*

In this issue, you will find articles describing our new safety partnership with Dow Chemical Company; some major new research center grants supporting theoretical chemistry efforts; a particularly exciting discovery from the Hoye research group that has garnered international attention; and profiles of a few of our outstanding students.

The safety partnership with Dow is already reaping major dividends. We are improving our culture of safety through a myriad of initiatives led by a group of graduate students and postdoctorates from our department and the Department of Chemical Engineering and Materials Science.

Research is thriving, as illustrated by increased levels of funding and the extensive dissemination of exciting new findings. Examples include the funding of two new theoretical chemistry centers led by Professors Christopher Cramer and Laura Gagliardi through new grants totaling more than $13 million from the Department of Energy; a serendipitous discovery of a useful new variant of the iconic Diels-Alder reaction by Professor Thomas Hoye and his research group; and a selection of other advances from the research groups of Professors Marc Hillmyer, Connie Lu, Valerie Pierre, and Andreas Stein.

Undergraduate participants in research gain greatly from their experiences, as shown in stories about two of our outstanding graduates, Spencer Knight and Julian Lo, who have gone on to enter doctorate programs. Updates on (many!) student and faculty honors round out the issue, including a story on Professor Christy Haynes being named one of *Popular Science's* "Brilliant 10."

Finally, please join me in welcoming new faculty member, Professor Will Pomerantz, whose research focuses on using $^{19}F$ spectroscopy to elucidate protein structure. As undergraduate enrollments in the College of Science & Engineering continue to increase, we are excited about growing our faculty. Our outstanding faculty members are committed to tackling the most critical scientific and educational challenges. Please stay in touch, and think about supporting our efforts to educate students and generate new knowledge.

# Kolthoff inducted into Science & Technology Hall of Fame

*One of the University of Minnesota's most famous chemists, Isaak Maurits Kolthoff, received, posthumously, a 2012 Tekne Award and was inducted into the Minnesota Science & Technology Hall of Fame.*

Isaak Kolthoff

The Tekne Award was created by the Minnesota High Tech Association to honor people whose achievements in science and technology have made lasting contributions to the state of Minnesota and to the world. The Minnesota Science & Technology Hall of Fame is a permanent exhibit at the Science Museum of Minnesota.

Isaak Kolthoff was a highly influential chemist. He is widely considered to be the father of analytical chemistry, developing it into a modern science. He was born on February 11, 1894, in Almelo, Holland. He died on March 4, 1993, in St. Paul, Minnesota. In 1911, he entered the University of Utrecht, Holland, where he earned his doctorate in chemistry. On the basis of his world-renowned reputation, he was invited to join the faculty of the University of Minnesota's Department of Chemistry in 1927. By the time of his retirement from the university in 1962, he had published approximately 800 papers. He continued to publish approximately 150 more papers until his health failed. He also was the author of textbooks and a 30-volume treatise on analytical chemistry.

Best known to the general public is Kolthoff's work on synthetic rubber. During World War II, the government established a comprehensive research program at major industrial companies and several universities, including Minnesota. Kolthoff quickly assembled a large research group and made major contributions to the program.

Kolthoff's research, covering approximately a dozen areas of chemistry, was recognized by many medals and memberships in learned societies throughout the world. He received honorary Doctor of Science degrees from the University of Chicago, the University of Groningen, Brandeis University, and the Hebrew University of Jerusalem. He was knighted by the Netherlands Government as a Commander in the Order of Orange-Nassau. He received the William H. Nichols Medal in 1949, the Robert Boyle Medal from the Royal Society of Chemistry in England, the Charles Medal of the Charles University in Prague, and the Fisher Award, among other awards and medals. In his honor, the University of Minnesota Board of Regents named a new chemistry research building Kolthoff Hall in 1972. In 1983, he received the America Chemical Society Division of Analytical Chemistry inaugural Award for Excellence in Teaching.

Many of Kolthoff's graduate students went on to successful careers in industry and academic life and, in turn, trained many more. In 1982, it was estimated that approximately 1,100 Ph.D. holders could trace their scientific roots to Kolthoff. The Department of Chemistry honors Kolthoff's legacy with the Kolthoff Lectureship in Chemistry, annually inviting some of the most renowned scientists in the world to present a series of lectures and meet with faculty members and students.

## William Pomerantz joins Department of Chemistry faculty

William Pomerantz

William "Will" Pomerantz, Ph.D., has joined the Department of Chemistry as an assistant professor.

Before coming to the University of Minnesota, Pomerantz was a National Institute of Health National Research Service Award postdoctoral research fellow at the University of Michigan. He earned his doctorate in organic chemistry from the University of Wisconsin-Madison; was a Seydel/Fulbright Fellow at the Swiss Federal Institute of Technology; and received his bachelor's degree in chemistry from Ithaca College.

Pomerantz is interested in modulating the function of protein-protein interactions through the use of small molecules and bio-inspired peptide scaffolds. His research uses organic synthesis, biophysical, biochemistry and molecular biology techniques to investigate the folding/misfolding and disease pathways of intrinsically disordered proteins (IDPs). His research interests exploit the bio-orthogonality and the hypersensitivity of fluorine chemical shifts to changes in chemical environment for probing important protein-protein interactions of structurally challenging proteins and to ultimately explore their behavior in cells (in-cell nuclear magnetic resonance). This research is complemented with established biophysical techniques, organic synthesis of chemical probes, and new peptide-based strategies for pre-organization and cellular delivery for studying challenging IDPs under physiological conditions.

# Undergraduates benefit from laboratory research experiences

*The Department of Chemistry's undergraduate program attracts some of the brightest students at the university. They excel in the chemistry academic program and in research, and some go on to attend excellent graduate schools. Two outstanding graduates are Spencer Charles Knight and Julian Castro Lo. Both graduated with the high distinction of summa cum laude in the spring of 2012.*

## Spencer Charles Knight

Spencer Charles Knight

Spencer is a first-year chemistry graduate student at the University of California, Berkeley, where he is conducting research under the tutelage of Professor Christopher Chang. His honors and awards at the University of Minnesota included a National Science Foundation Graduate Fellowship, a College of Science & Engineering Merit Scholarship, an Undergraduate Research Opportunities Program grant, a Heisig/Gleysteen Summer Research Fellowship, and a Prentice Hall Organic Chemistry Book Prize. Under the tutelage of his advisers, Professors William Tolman and Marc Hillmyer, Spencer wrote an honors thesis titled, "Mechanistic Studies of Indium Catalysts for the Polymerization of Lactide and Synthesis of Biorenewable Polyols from Carvone."

Spencer enjoyed his undergraduate laboratory experiences.

"Working in Bill Tolman's lab was a blast!" he said. "Some of my favorite experiences were using the outstanding instrumentation facilities at Minnesota, including the nuclear magnetic resonance lab, the characterization facility, the mass spectrometry facility, and various instruments in the Tolman and Hillmyer labs; creating testable plastic films from the polymers that I synthesized in lab; and sharing my research at conferences, undergraduate poster sessions, and even the Minnesota State Fair."

Learning from graduate students and postdoctoral researchers was an important part of his undergraduate experiences.

"I thoroughly enjoyed interacting with all of the great graduate students and postdocs in the Tolman and Hillmyer groups over the years," he said. "They greatly improved the quality of my science, helped me to develop critical thinking skills, and made life in the lab a lot more fun."

Those laboratory experiences taught Spencer some fundamental laboratory techniques and improved his critical-thinking skills.

"I learned how to dig through the literature when tackling brand new scientific problems, and how to design appropriate experiments when things go wrong," said Spencer. "I also learned the value in collaborating with others to solve problems."

Spencer's current research is focused on developing chemical probes for imaging iron in neurons. Elucidating the mechanisms of iron signaling and trafficking in the brain might lead to a better understanding of how neurodegenerative diseases, aging, and memory work at the molecular level.

His experiences in the chemistry program at the University of Minnesota are propelling him toward a possible future as a professor at a research university.

"I am passionate about teaching, and I also really enjoy research," he said. "I would ideally like to be a professor at a research university one day. For the time being, I am content with just surviving and doing well in my first semester of graduate school."

## Julian Castro Lo

Julian Castro Lo

Julian Castro Lo, a first-year graduate student at The Scripps Research Institute (TSRI) in La Jolla, CA, is seeking a doctorate in organic chemistry, and is conducting research under the tutelage of Professor Phil Baran.

While at the University of Minnesota, he received many prestigious scholarships, fellowships, and awards, including a National Science Foundation Predoctoral Fellowship, the David A. and Merece H. Johnson Scholarship, the Pfizer La Jolla Academic-Industrial Relations Diversity Research Fellowship in Chemistry, the Brasted Memorial Fellowship, the Heisig/Gleysteen Summer Research Fellowship, the Undergraduate Research Opportunities Program Award, the American Chemical Society Division of Inorganic Chemistry Undergraduate Award, the J. Lewis Maynard Memorial Prize in Advanced Inorganic Chemistry, and the Merck Index Award.

Julian conducted research in the Professor Thomas Hoye's laboratory. What he learned working with the Hoye research group is helping him at Scripps.

"Working on a natural product synthesis in the Hoye group gave me the opportunity to familiarize myself with numerous reactions and to work with a myriad of different reagents," said Julian. "I've run several of those same reactions at Scripps. The very first reaction I ran in graduate school was one that I had run

many times as an undergrad. As lame as this might sound, performing familiar chemistry at a time when everything else was unfamiliar washed away my anxiety about starting graduate school."

Beyond the research experiences, Julian said that the highlights of his undergraduate research were the daily interactions with other members of Hoye's research team.

**"They showed me what it means to be a successful chemist: the curiosity that leads one into the unknown…"**

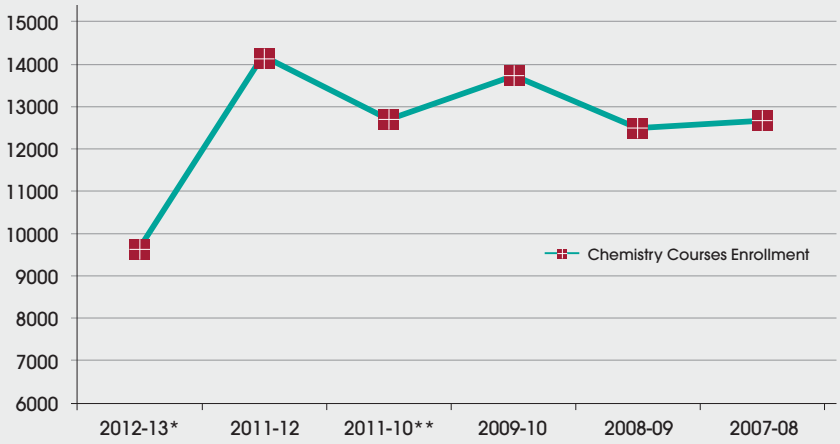
*—Julian Lo*

"They taught me everything that I know about laboratory techniques from things as simple as evaporating off solvent using a rotovap to pretty challenging things such as working with compounds that decompose upon touching air," said Julian. "They showed me what it means to be a successful chemist: the curiosity that leads one into the unknown; the self-discipline that allows one to keep chugging along when success is rare; and the ability to keep one's composure when the unexpected happens. Everyone in the group had some role, direct or indirect, in mentoring me and I will always cherish my memories of them."

Julian's research in the Baran laboratory at The Scripps Research Institute centers on using natural product synthesis as a platform to explore chemical reactivity and develop innovative solutions to current deficiencies in organic chemistry. Currently, he is working on a total synthesis of a family of terpene natural products via a biomimetic route that involves the construction of an archetypical carbon skeleton of the family and subsequent oxidation utilizing a variety of C-H functionalization and other techniques to arrive at the desired family members.

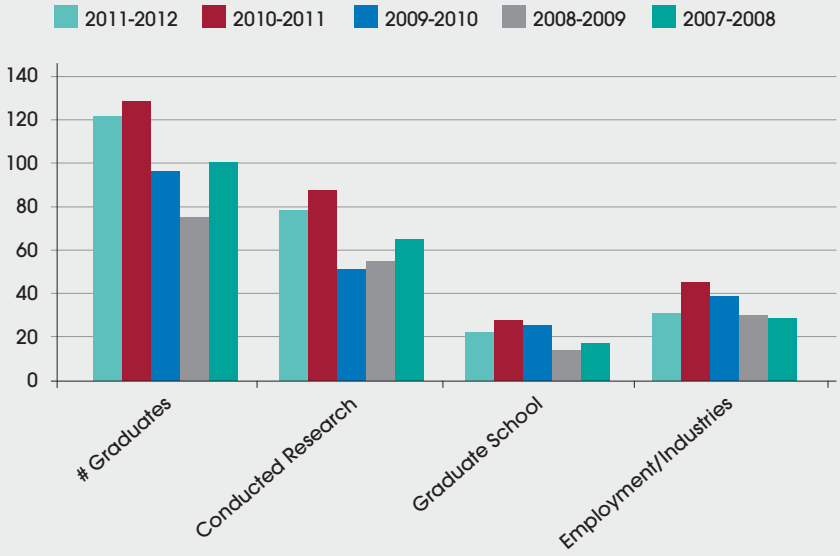
As for the future, Julian wants to pay his mentorship experiences forward. "Given all my positive experiences being mentored, I would like to eventually start my own research group at a university and mentor younger generations of chemists," he said. "Making it through graduate school would be a good first start though!"

## Chemistry Courses Enrollment




Chemistry has some of the highest enrollments in the College of Science & Engineering and the University of Minnesota. Most undergraduates are required to take general chemistry courses. *The 2012-13 enrollment only includes the number of enrolled students for the fall of the 2012-13 school year. **The 2010-11 enrollment does not include the number of students enrolled during the summer.

## Our Undergraduates: By the Numbers




Each year a high percentage of Department of Chemistry undergraduates participate in research opportunities. This chart illustrates the number of graduates, the number of students that conducted research, and their self-reported plans for graduate school or employment in industries.

# Researchers uncover the broad scope

*"Serendipity—discovering by accident something good or useful that was not being searched for." It is not surprising that serendipity occurs a lot in the scientific community. But it takes curiosity, knowledge, wisdom, and tenacity to prevent that serendipitous discovery from being overlooked or dismissed as a mistake.*

Professor Thomas Hoye

Professor Thomas Hoye and members of his research team have uncovered the heretofore-overlooked scope of an important chemical reaction, which they have named the hexadehydro-Diels-Alder (HDDA) reaction. Discovering new modes of chemical reactivity is rare and is so unprecedented that the University of Minnesota is seeking a patent for it.

Hoye's reaction builds on the work of Otto Paul Hermann Diels and Kurt Alder, who first documented what is called the Diels-Alder reaction in 1928. They received a Nobel Prize for their work in 1950. Every chemist knows about the Diels-Alder reaction. It is presented in every chemistry textbook and taught to every organic chemistry student.

The new HDDA reaction is a variant of that classic Diels-Alder reaction (Figure 1). In the typical Diels-Alder reaction, six-membered rings (cyclohexenes, **3**) are formed by the reaction of two precursors—a diene (1) and a dienophile (**2**). The hexadehydro-Diels-Alder reaction involves, instead, the cycloaddition of a conjugated diyne (**4**) with another alkyne, the "diynophile" (**5** ). But this seemingly subtle difference has a huge, beneficial ramification. The product is, itself, a highly reactive species called a benzyne (**6a/6b**).

Benzynes are one of the most widely studied and useful of all "reactive intermediates" encountered in organic chemistry. However, because of the preparative requirements for generating benzynes, they can be challenging to make. In addition, because of the other external reagents, which are other additives needed to bring about chemical reactions, and byproducts such as metals and bases that accompany the typical methods for preparing benzynes, certain types of benzyne trapping reactions are not feasible. In contrast, the two-stage HDDA cascade reaction (Figure 2) merely involves heating the appropriate triyne precursor (e.g., **7**) in the presence of the benzyne trapping agent; no other reagents need to be present. Thus, the HDDA process represents a highly complementary and orthogonal method for constructing the high-energy benzynes (e.g., **9**, enroute to **8** via **10**).

Benzynes are highly valued because of their remarkable efficiency and ability to react with other chemical substances. They are used to build structurally complex benzenoid products

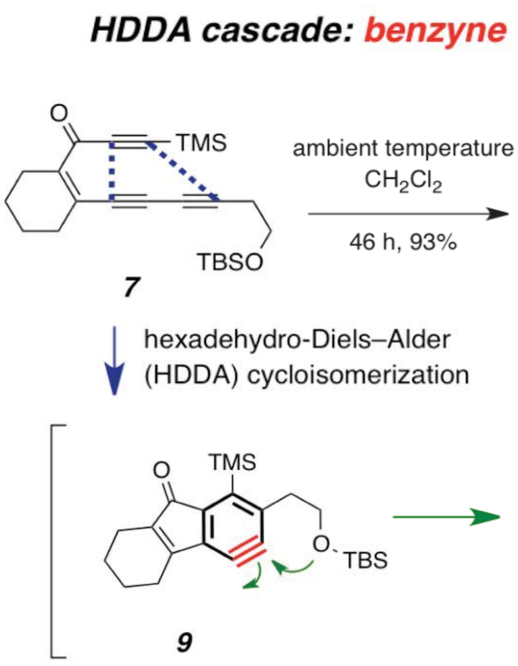



Figure 2

(cf. **8**), which are stable, versatile, synthetic organic compounds used in the development of pharmaceuticals, including many marketed drugs (i.e., pharmaceutical agents), agrochemicals, dyes, and polymers.

Postdoctorate researcher Beeraiah Baire, Ph.D., unexpectedly encountered the first example of the HDDA reaction during the course of an unrelated study in July 2011.

"We could have easily talked ourselves out of this," said Hoye. "We sensed that we were on to something, but we initially didn't know what

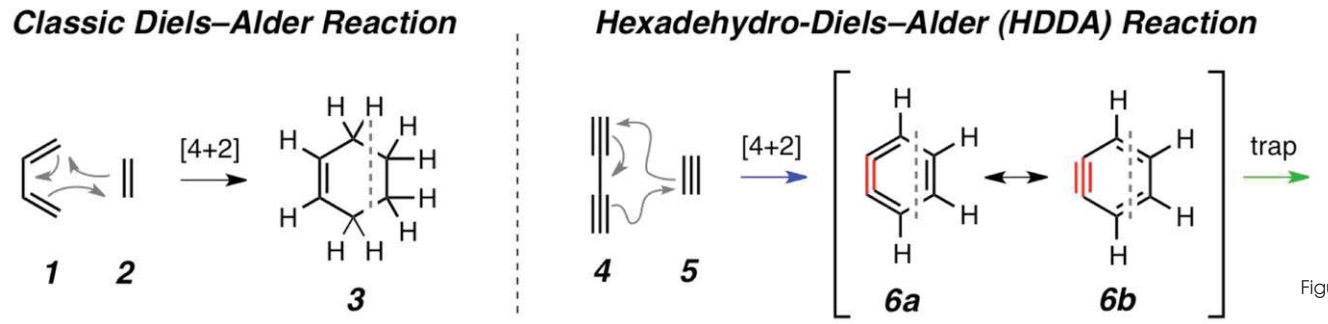
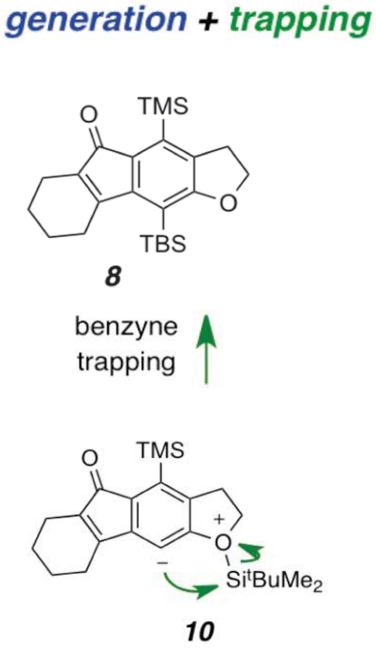



Figure 1

# of overlooked chemical reaction




it was. Something instinctively told us that this was an important observation and discovery."

**"We could have easily talked ourselves out of this… Something instinctively told us that this was an important observation and discovery."**

*—Professor Thomas Hoye*

Since last summer, Hoye, Baire, and graduate students Dawen Niu, Patrick Willoughby, and Brian Woods have been using the HDDA reaction to create benzynes and have been studying the resulting new reactivity patterns. Hoye hopes that this ongoing research will lead to new discoveries for the use of benzynes. One example is the development of compound libraries useful to support drug discovery efforts.

Their work on the hexadehydro-Diels-Alder reaction was published in the October 11 edition of *Nature* (doi:10.1038/nature11518).

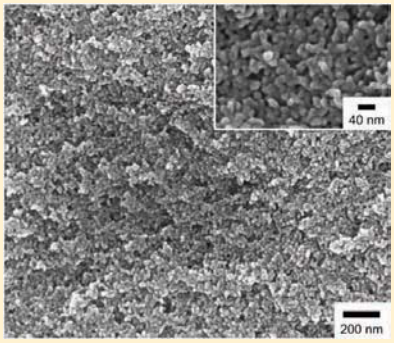
Hoye is a top organic chemist and professor. He joined the University of Minnesota chemistry faculty in 1976 and has received accolades for his research and his teaching, including being named the Merck Professor of Chemistry in 2002, being recognized as a Distinguished Graduate Teaching Professor in 1999, and receiving the Horace T. Morse University of Minnesota Alumni Association Award for Outstanding Contributions to Undergraduate Education in 2007. More than 130 undergraduates students have done independent research studies in his laboratories. Twelve masters and 74 doctoral graduate students have carried out their thesis research under his guidance, and dozens of postdoctoral and visiting scientists have studied in his group.

The primary emphasis of Hoye's research group is the development of new strategies for natural product total synthesis.

## Bicontinuous Nanoporous Plastics by a Simple Process

*Professor Marc Hillmyer and postdoctoral researcher Myungeun Seo, Ph.D.*

A method of generating reticulated nanoporous polymers using a simple process that holds tremendous promise for many applications in nanoscience and technology. By incorporating a crosslinker in the controlled polymerization process for block polymer synthesis, Seo found that microphase separation occurs during polymerization and produces a crosslinked nanostructured composite with bicontinuous morphology. Reticulated nanoporous polymers with sub-10 nm pores were readily obtained by selective etching of a sacrificial segment. A scanning electron microscope (SEM) image of a typical nanoporous sample is shown below. Combining the advantages of block polymer self-assembly and polymerization-induced phase separation presents a simple way to make nanoporous polymers with pores percolating in 3D, precise control over pore size distribution, and mechanical integrity. The report describing this work was published in the journal *Science*.

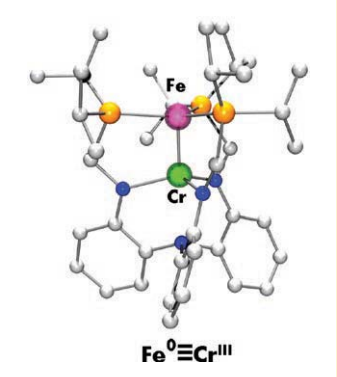



A representative scanning electron micrograph of reticulated nanoporous polymer after ~ 1 nm of Pt coating (inset: magnified image)

## Going Short with Iron and Chromium

*Professors Connie Lu and Laura Gagliardi, graduate student P. Alex Rudd, undergraduate Shengsi (Mike) Liu, and postdoctoral researcher Nora Planas, Ph.D.*

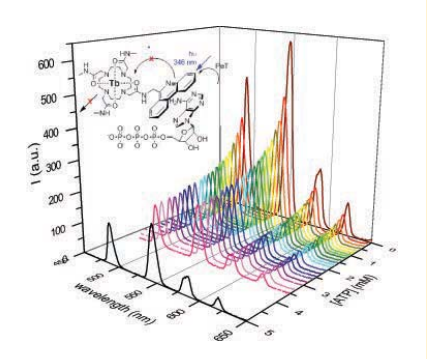
Transition metal pairs can form multiple bonds with versatile, multi-electron redox properties, which is promising for catalytic applications. A wide range of unique electronic properties and chemical reactivity can be imagined for the vast combinations of first-row TM elements in their various oxidation states. Using a "double-decker" ligand that can bind two transition metals together, Lu and Rudd have bonded iron to chromium in an ultra-short way: the metal-metal bond length is less than 2 angstroms (1.94 Å)! Their molecule is the first example of multiple bonds between different first-row metals and broke the record for the shortest heterobimetallic bond. Gagliardi, Liu, and Planas performed the quantum chemical calculations that revealed a formal triple bond and elucidated the metal oxidation states as zero-valent iron and Cr(III). This work has been submitted to *Angewandte Chemie*. Ultimately, this research aims to understand how one transition metal influences another, with the ultimate goal of tuning chemical properties and reactivity by the scholarly choice of metal-metal pairings. Currently, the researchers are studying the reactivity with carbon dioxide in gearing towards catalytic $CO_2$ conversion.




## A Selective Luminescent Probe for the Direct Time-Gated Detection of ATP

*Professor Valerie C. Pierre, graduate student Evan A. Weitz, and undergraduate students Jennifer Y. Chang and Adam H. Rosenfield*

Kinases, enzymes that transfer a phosphate groups from adenosine-5′-triphosphate (ATP) to specific protein substrates, currently represent one of the two largest classes of targets for drug discovery. The search for new kinase inhibitors, critical tools in cancer therapy, often begins with the high throughput screening of libraries followed by the evaluation of the potency of potential leads and their selectivity for a desired kinase. These studies require the widespread availability of efficient and affordable screens for kinase activity. The most important features coveted by researchers in a probe are that the probe must concurrently be affordable, non-radioactive, label-free, antibody-free, generic (able to screen all classes of kinases), and must enable the study of large protein substrates. In addition time-resolved or time-gated luminescence detection is highly preferred as are assays that measure the accumulation of ADP as opposed to the phosphorylation of a peptide or the displacement of a biomarker. None of the current commercial assays fulfill all of these requirements.

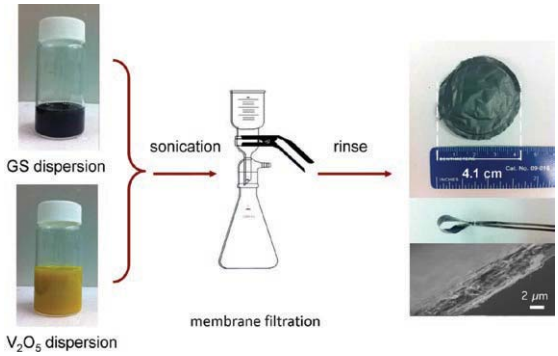



Moreover, none can be performed at higher concentrations of ATP, closer to the intracellular concentrations of 1-10 mM needed to study inhibitors of low-affinity kinases, and none enable direct real-time monitoring of kinase kinetics. Through rational design, the Pierre research group has recently developed the first luminescent probe that fulfills all user-defined requirements. The probe consists of a small terbium complex that binds reversibly and with differential affinity ATP, adenosine diphosphate (ADP) and adenosine monophosphate (AMP). The probe is designed in such a way that binding of the nucleotide affects its luminescence; the different binding affinities thus advantageously enable direct monitoring of enzymatic reaction. This work was published in the *Journal of the American Chemical Society.*

## Flexible Battery Electrodes from Nanoparticles

*Professor Andreas Stein and graduate students Yuqiang Qian and Anh Vu*

Due to the growing interest in flexible electronics such as roll-up displays, stretchable integrated circuits, and wearable multimedia or medical devices, there is a need to develop rechargeable batteries with flexible structures by commercially viable methods. To achieve this goal, graduate students Yuqiang Qian and Anh Vu devised a straightforward preparation of composite electrode films from vanadium oxide ($V_2O_5$) nanowires and graphene nanosheets. $V_2O_5$ has been widely studied as an electrode material for rechargeable lithium batteries due to its low cost and high energy density. However, its electrical conductivity is limited, and it is typically used in the form of a powder. When $V_2O_5$ is normally employed in an electrode, it therefore requires additives such as conductive carbon particles and a binder. By simply mixing water-based dispersions of graphene nanosheets (GS) and $V_2O_5$ nanowires and passing them through a filter, free-standing, flexible $V_2O_5$-graphene composite films were prepared, suitable as binder-free electrodes in lithium ion batteries.




The use of a surfactant in the synthesis mixture facilitated good dispersion of the two nanoparticle components in water, ensuring good intermixing of them in the composite films. The electrical conductivity increased with higher loadings of graphene nanosheets, which provided an electron pathway. The integrated composite structure, composed of flatly-aligned, crystalline $V_2O_5$ nanowires embedded within stacks of graphene sheets, endowed the films with excellent charge and discharge properties, good cyclability, and, depending on the relative $V_2O_5$:GS content, high specific capacity and/or high rate capabilities. Because the $V_2O_5$:GS ratio can be easily adjusted during the film synthesis, it can be optimized for specific rate or capacity requirements. These composite films are promising candidates for electrical energy storage applications that require flexible electrodes. This research was published in the *Journal of the Electrochemical Society.*

# Awards enable collaborations with undergraduate institutions

The National Science Foundation (NSF) made two awards to support research teams led by Professor Ilja Siepmann and co-investigators at primarily undergraduate institutions (PUIs). The co-investigators are Department of Chemistry alumni.

The award from the Division of Chemical, Bioengineering, Environmental, and Transport Systems is aimed at the development of transferable force fields and efficient Monte Carlo algorithms and their application to phase and sorption equilibria. This collaboration involves Professor Becky Eggimann and her students at Wheaton College who will spearhead the design of an interactive web page for the transferable potentials for phase equilibria (TraPPE) force field.

The award from the Chemistry Division is aimed at the development and application of Monte Carlo simulation tools for hydrophilic interaction liquid chromatography, ion chromatography, and surface enhanced Raman spectroscopy (SERS) chemosensors. This collaboration involves Jake Rafferty at North Hennepin Community College. He will analyze simulation trajectories.

In addition to the PUI researchers, these projects also benefit from collaboration with Peter Koenig at Procter & Gamble and Mark Schure at Dow Chemicals.

Since 2010, Siepmann has been heading a collaborative project supported by an NSF Cyber-enabled Discovery and Innovation grant aimed at providing molecular-level understanding of atmospheric nucleation projects. This project involves Kelly Anderson at Roanoke College.

Eggimann, Rafferty and Anderson are all Department of Chemistry alumni who conducted their graduate research at the University of Minnesota.

## Laboratory safety efforts *continued from page 1*

opportunity for universities everywhere," said Pankaj Gupta, Ph.D., senior strategy leader for research and development at Dow Chemical Company, who along with others on the Dow team has been collaborating with the two U of M departments. "Through this safety partnership with the University of Minnesota, we expand our relationship by leveraging our strength in laboratory safety," he said.

This safety partnership will benefit the University of Minnesota and has the potential to help other universities across the country as well.

Graduate students and postdoctoral researchers in the two departments have formed a Joint Safety Team (JST), which comprises 62 Laboratory Safety Officers (LSOs) and a number of interested graduate students from the two departments.

The JST's safety campaign focuses on four key areas—**CARE**:

- **Compliance:** improve compliance with lab standards on hazardous waste handling, sample and chemical storage, lab cleanliness, and the wearing of personal protective equipment (PPE);
- **Awareness:** improve awareness of safety hazards, best practices, and available resources around the theme of "Safety Starts with U!";
- **Resources:** improve the quality of and access to safety resources, including the standardization of laboratory signs, development of safety websites, and PPE such as goggles, lab coats, and gloves; and
- **Education:** improve the training and ongoing education of laboratory safety officers and researchers.

The JST has developed a number of short-term and long-term recommendations for improving safety practices. These recommendations will act as a guidebook to improving the safety culture at the university.

> **"We identified areas of safety that needed improvement and devised a list of ways to address those areas."**
>
> *—Kathryn "Kate" McGarry, CHEM graduate student and JST Administrative Committee chair*

"We identified areas of safety that needed improvement and devised a list of ways to address those areas," said Kathryn "Kate" McGarry, a CHEM graduate student and chair of the JST Administrative Committee. "The JST will be working closely with our department chairs, personnel from the University's Department of Environmental Health & Safety (DEHS), and members of Dow Chemical Company to implement these recommendations. Our motivation and actions hopefully will encourage the rest of our community to join us in establishing a better culture of safety," she said.

The short-term recommendations were implemented this fall. They include creating and posting new laboratory signs that emphasize PPE requirements, potential hazards in the lab, and guidelines on how to make the laboratories safer places to conduct research. "Safety Starts with U!" posters were created and are strategically posted in the departments.

Other plans include conducting Safety Moments at the start of all departmental seminars and group meetings; publishing Safety Notes in the departments' weekly email newsletters; conducting the first-ever departmental cleanup week; writing, evaluating, and sharing laboratory-specific safe operating procedures; and sending monthly emails on safety learning experiences.

Long-term, the JST will focus on maintaining the safety campaign.

"This campaign addresses the need to improve the culture of safety in our laboratories in proactive, collaborative, and direct ways," said Professor William Tolman, chair of the Department of Chemistry. "The fact that it is being led by the graduate students and postdoctoral researchers is terrific. Their energy and creative ideas are already having a profound impact," he said.

What is learned in this pilot project could be shared across the university.

"The Department of Environmental Health and Safety is committed to learning from this innovative program and sharing what we have learned from this experience with others across the campus," said Craig Moody, director of the DEHS. "The students involved in this program should be very proud in knowing they will have an impact on the health and safety of thousands of students and staff in the years to come."

## Fellowships

**3M Science & Technology Fellowships**—Clay Easterday, Audrey Meyer, Christopher Roberts, Ivan Spector, and Stephen Tereniak

**ConocoPhillips Fellowship**—Zahra Sohrabpour

**Doctoral Dissertation Fellowships**—Yuanyan Gu, Brynna Jones, Benjamin Manning, Audrey Meyer, Dawen Niu, Nicholas Petkovich, and Bess Vlaisavljevich

**Lester C. and Joan M. Krogh Endowed Fellowship**—Christopher Huber

**Kenneth E. & Marion S. Owens Endowed Fellowship**—William Isley III

**National Science Foundation Graduate Student Fellowships**—Spencer Knight, Julian Lo, and Randall Siedschlag

**Wayland E. Noland Fellowship**—Mohammad Mohsen Mahmoodi

**Dr. Venkateswarlu Pothapragada and Family Graduate Fellowship Fund**—Mayank Puri

**Newman and Lillian Bortnick Fellowship**—Jennifer Soltis

**John Wertz Fellowship**—Benjamin Wilson

## Scholarships

**Auzins Scholarship**—Srijay Rajan

**Andrews Scholarship**—Dylan Walsh

**Robert C. Brasted Memorial Fellowship**—Alexander Nicol

**Thomas DuBruil Memorial Award**—Moriana Haj, Erin Hill, Megan Magee, Maximilian Margherio, and Quang Luu Nguyen

**Lloyd W. Goerke Scholarship**—Adam Matula

**David A. and Merece H. Johnson Scholarship**—Sam Kenny and Mark Strom

**George T. Walker Scholarship**—Hanna Erickson and Takanori Sagawa

## Individual Awards

**CRC Freshman Chemistry Achievement Award**—Sammy Shaker

**Barry M. Goldwater Scholarship**—Mark Strom

**J. Lewis Maynard Memorial Prize in Advanced Inorganic Chemistry Award**—Michelle Johnson

**Merck Index Award**—Dylan Walsh and Peter Stevens

**Undergraduate Award in Analytical Chemistry (ACS)**—Jason Brennan

**Wayland E. Noland Award for Academic Excellence in Chemistry**—Jua Choi

Recipients of the **Thomas DuBruil Memorial Award** were, from left, Maximillan Margherio, Moriana Haj, Megan Megee, Erin Hill, and Quang Luu Nguyen.

## Videos to enhance learning in organic laboratory course

Professor Jane Wissinger, organic lab director, received a $10,000 Office of Information Technology (OIT) Faculty Fellowship. She will use this fellowship to develop a series of videos encompassing apparatus, observations, and problem-solving skills for her organic laboratory course.

The videos will augment Wissinger's lectures, and reinforce proper experiment and laboratory techniques, and equipment and chemical use. Wissinger said that there are about 15 techniques, eight apparatus, and four instrument data interpretations taught throughout the semester-long course. Each video will include step-by-step details, hints, and suggestions. The videos will be posted on the web and easily accessible to students. They also will be used to train teaching assistants.

# Major grants fund important research and development of multi-institutional centers

*Research is at the center of what the Department of Chemistry does, generating new knowledge and teaching students. Researchers in the department address a variety of health, environment, energy, and next-generation technology issues. Each year, faculty members bring in millions of research dollars to the university to support their research. In 2011, the department had more than $17.5 million in active research grants.*

Collaborative projects are more important than ever for addressing some of the most challenging scientific problems, which are often uniquely interdisciplinary and multifaceted. A number of major grants received by chemistry faculty during 2011-2012 fund collaborative work with other researchers at the university and across the country. These grants provide critical funding in support of the department's postdoctorate researchers, graduate students, and undergraduate students. They also support the broader education of members of society about the importance of the research.

"Large multi-investigator grants play an ever increasing role in academic research," said William Tolman, department chair. "They are critical for tackling wide-ranging problems that cross traditional scientific boundaries, and they enable creative instructional initiatives to be pursued. Our success in garnering such support speaks to the outstanding leadership of our faculty in directing cutting-edge research and developing new educational programs," he said.

Christopher J. Cramer and Laura Gagliardi

## $13.1 million in Department of Energy funding for two new nationwide centers

The University of Minnesota has been awarded two grants from the U.S. Department of Energy (DOE) totaling $13.1 million over the next five years to fund two nationwide centers headquartered in the Department of Chemistry.

Research within the two centers will include developing new materials related to capturing greenhouse gases and improving chemical processes as well as developing methods and software tools for increasing the efficiency of solar energy conversion.

Both of these grants were competitive with many other institutions submitting proposals and only a handful chosen for each, said chemistry professors Laura Gagliardi and Christopher J. Cramer, who lead the university's two new centers. "It's rare to have two major DOE initiatives at the same institution, but the proposal reviews indicate that we were chosen because of our excellent researchers and the University's Minnesota Supercomputing Institute, which provides state-of-the-art computing facilities," Gagliardi said.

The **Nanoporous Materials Genome Center** will be funded with $8.1 million over five years as a DOE Center for Materials or Chemical Science Software Innovation. The center will develop and use high-end computational tools to characterize and predict the performance of millions of advanced materials at the nano scale. These new materials have many potential applications related to energy, including the capture of greenhouse gases, such as $CO_2$, and the storage of hydrogen. In addition, the group aims to improve catalysis and advanced chemical separations used in environmental research, as well those used in petroleum and biofuels processes to make them more efficient and environment-friendly.

The Nanoporous Materials Genome Center will be based at the University of Minnesota and include researchers from six other institutions including the University of California, Berkeley; Lawrence Berkeley National Laboratory; Washington State University; Rice University; Georgia Tech; and Northwestern University. Gagliardi will serve as this center's director.

"It's wonderful opportunity for us to collaborate with our colleagues nationwide to make significant contributions in important areas of environmental research," Gagliardi said.

The **Center for the Study of Charge Transfer and Charge Transport in Photoactivated Systems** is funded by a $5 million grant over five years through the DOE Scientific Discovery through Advanced Computing (SciDAC) initiative. Researchers will develop methods, algorithms, and improve software tools needed for the reliable modeling of charge transfer and charge transport in photoactivated systems. Such processes are fundamental for solar energy capture, solar energy conversion, and photoactivated catalysis, both industrial and biological. Cramer will serve as center director.

Research partners include Pacific Northwest National Laboratory and Lawrence Berkeley National Laboratory.

"The computational chemistry group at the University of Minnesota is world-class, with an outstanding record of accomplishments," said Tolman. "Their expertise in theory development and applications is second to none, putting them in a great position to make significant research progress on the critical problems targeted by the DOE center grant proposals."

In addition to Gagliardi and Cramer, other participating University of Minnesota faculty members involved in the centers include chemistry professors Donald G. Truhlar and J. Ilja Siepmann, and chemical engineering and materials science professor Michael Tsapatsis. Cramer, Gagliardi, Siepmann, and Truhlar are members of the department's Chemical Theory Center.

## Center for Sustainable Polymers

The Center for Sustainable Polymers (CSP) is focused on harnessing renewable, functional, degradable, and non-toxic ingredients from nature for tomorrow's advanced plastics, foams, adhesives, elastomers, coatings, and other macromolecular materials.

The CSP was launched in 2009 with seed funds from the University's Initiative for Renewable Energy & the Environment large-grant program. Last year, the CSP received a phase I, $1.5 million, three-year grant from the National Science Foundation Center for Chemical Innovation (CCI) program. The CSP is now eligible for a phase II grant that could provide up to $40 million over 10 years. Professor Marc Hillmyer is the center's director.

Professor Marc Hillmyer

In addition to its focus on sustainable polymeric materials, the CSP fosters partnerships with industry leaders, and develops outreach activities designed to educate future scientists and the public about the science and technology of sustainability.

CSP researchers have made bold scientific advances in the areas of catalysis, plastics and elastomers, and polyols, including:

- Developing several new renewable polyester and polyether polyols for thermoplastic and thermosetting polyurethanes. These new polyurethane structures are possible replacements for petroleum-based systems and products, ranging from elastomers to adhesives.
- Discovering a simple and efficient method for the conversion of carboxylic acid containing molecules derived from biomass into olefins through a catalytic decarbonylation process.
- Discovering and developing new renewable thermoplastic elastomers using a combination of controlled polymer synthesis techniques. These materials have shown outstanding mechanical performance.

This year, the CSP funded two seed projects. Professors Kechun Zhang and Yiannis Kaznessis from the Department of Chemical Engineering and Materials Science are engineering microbes that synthesize renewable and cost-effective methyl-substituted lactones from glucose. Professor Claudia Schmidt-Dannert from the Department of Biochemistry, Molecular Biology and Biophysics, and Professor Mark Distefano from the Department of Chemistry hope to develop a microbial and biacatalytic *in vitro* production system for rubber.

The CSP is engaged in a number of outreach activities, including:

- Training high school teachers from Minnesota, New York, and Georgia on a new laboratory experiment in which students make bioplastic from starch (potato, tapioca, or corn), add an additive to manipulate the plastic's properties (glycerol or sugar) and then test those properties.
- Working with the Center for Science, Technology, and Public Policy (CSTPP), LifeScience Alley, and the BioBusiness Alliance of Minnesota to sponsor site visits to biochemical companies such as Nature-

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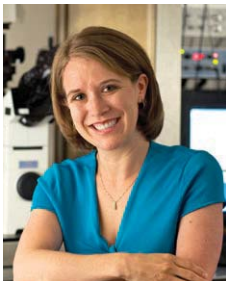
# Professor Haynes named one of *Popular Science's* 'Brilliant 10'


Professor Christy Haynes

**Professor Christy Haynes** has been named one of *Popular Science* magazine's "Brilliant 10," an honor that recognizes an elite group of young scientists whose research is expected to dramatically impact their fields.

Haynes has been working with her research group to study blood platelets. Platelets are small, irregularly shaped cell fragments that circulate in the blood and are an essential component of blood clotting. Platelets are about one-tenth the size of average cells in mammals. They have proven difficult to study due to their small size and their biological function to react immediately when in a foreign environment.

"Platelets are really 'sticky' types of cells because they are used in clotting so it makes them difficult to study," Haynes said.

Haynes and her team are the only researchers in the world who have been able to measure chemicals being released by individual platelets in real time. They were the first to successfully isolate an individual platelet under a microscope, place a minuscule electrode onto it, and measure the messenger molecules released.

Understanding how platelets communicate with each other gives researchers fundamental knowledge that they never had before. This could lead to new treatments for patients who have difficulty with blood clotting or developing medications to help patients avoid dangerous blood clots.

Haynes is already collaborating with renowned platelet specialists nationwide to look at platelet samples and conduct initial lab testing for possible anti-clotting medicines.

"Being chosen as one of *Popular Science's* Brilliant 10 brings new recognition to the graduate students on my research team and my fellow researchers to show that there is big science and big thinking going on here at the University of Minnesota," Haynes said.

Haynes and her colleagues recently formed the Center for Analysis of Biomolecular Signalling within the University of Minnesota Department of Chemistry. The research will be focused on learning more about how cells in the body send chemical signals to each other during immune response, blood clotting, muscle firing and more.

In addition to studying platelets, Haynes has been building "an immune system on a chip," where she is isolating and studying the various way cells communicate and respond to each other. With more information about how immune cells interact, she helps to open new avenues for treating allergic reactions and asthma.

Haynes' profile was published, Tuesday, September 11, on the PopSci website and was featured in the *Popular Science* magazine.

## Stanley Bonnema

**Stanley Bonnema**, retired senior administrative director, received a 2012 *President's Award for Outstanding Service*. This prestigious award honors current and retired employees who have gone well beyond their regular duties and who have demonstrated unusual commitment to the university community. Bonnema served as the senior administrative director for the Department of Chemistry for 31 years before his retirement in June 2009. Before that, he was senior lab service coordinator and chemistry laboratory supervisor for eight years.

## Two professors receive CAREER awards

Two assistant professors—**Christopher Douglas** and **Valerie Pierre**—have received CAREER awards from the National Science Foundation (NSF). The Faculty Early Career Development (CAREER) Program is one of the NSF's most prestigious awards. It supports junior faculty who exemplify the role of teacher-scholars through outstanding research, excellent education, and the integration of education and research within the context of the mission of their organizations.

Douglas' research encompasses discovering new chemical synthesis methods involving the metal-promoted activation of carbon sigma bonds in ketones, esters, and aldehydes. A major focus will be on the insertion of unsaturated groups into the activated bonds. Mechanistic work will be undertaken to develop a deeper understanding of the new reactivity develop. The methods developed will be applied to a diverse set of synthesis challenges. Applications will range from the synthesis of commodity chemical feedstocks like methyl ethyl ketone to the synthesis of complex natural products.

Pierre's research focuses on luminescent lanthanide probes for biological imaging of metal ions. This approach employs the coordination of chemistry and the unique photophysical properties of lanthanide complexes as components in a predictive design strategy in the development of new sensors for group I ions, and the application of these sensors in cellular imaging. The ultimate goal is to produce new tools enabling the simultaneous and selective spatio-temporal imaging of multiple alkali cations in tissues. This work advances the field of lanthanide chemistry by investigating the electronic and geometric requirements of their sensitized luminescence, and the field of molecular recognition by investigating novel binding modes.

## Three chemistry researchers honored for their inventions

Three professors—**George Barany**, **Philippe Buhlmann**, and **Marc Hillmyer**—were honored at the *University Innovations 2012* celebration event. Sponsored by the Office of the Vice President for Research, Univer-

sity Innovations 2012 honored researchers whose work has been patented, licensed to a company, or used to form a start-up company. Barany was honored for his patent, *Detection of Nucleic Acid Sequence Differences Using the Ligase Detection Reaction with Addressable Arrays*. Buhlmann was honored for his license, *Chemical Sensors Based on Fluorous Sensing Membranes*. Hillmyer was honored for his license, *Fabrication of Robust Nanoporous Polymer Films with Cocontinuous Structures.*

## Christy Haynes

**Professor Christy Haynes** has been awarded the *New Orleans Kavli Foundation Emerging Leader in Chemistry Lecture* by the American Chemical Society Multidisciplinary Program Planning Group. As recipient of this award, Haynes will deliver a lecture on her research during the ACS National Meeting in New Orleans in April 2013. Her lecture will focus on biological and ecological toxicity in engineered nanomaterials.

Haynes is an emerging leader in the areas of nanoparticle toxicity and nanotherapeutics. She has pioneered the technique of carbon-fiber microelectrode amperometry to study the effect of nanoparticle uptake on cellular physiology.

## Marc Hillmyer

**Professor Marc Hillmyer** was named a *2012 Poly Fellow* of the American Chemical Society's Division of Polymer Chemistry, Inc. Fellows are nominated by their peers, and are honored for their outstanding achievements and contributions to polymer science and the profession.

Hillmyer teaches polymer, materials, organic, physical, and environmental chemistry. His research interests encompass the design, synthesis, and applications of functional polymeric materials, particularly polymers made from renewable resources, and the use of block polymers to prepare nanoporous materials for applications in water purification, advanced lithography, and solar energy conversion. He is director of the university's Center for Sustainable Polymers, which integrates science, technology, and public policy initiatives and research aimed at reducing dependence on petrochemicals for the creation of plastics.

## Alden Mead

**Professor Emeritus C. Alden Mead** won the *2012 Wigner Medal*. Mead was honored for his work on the gauge theory of molecules and its application to molecular spectra and scattering. He was a professor of physical chemistry in the Department of Chemistry from 1958 to 1993. The Group Theory and Fundamental Physics Foundation established the Wigner Medal in 1977, honoring scientists for their outstanding contributions to the understanding of physics through group theory.

## Theresa Reineke

**Professor Theresa Reineke** received a *2012 Outstanding New Investigators Award from the American Society of Gene & Cell Therapy (ASGCT)*. Reineke was honored for her contributions to the field of gene and cell therapy. She is one of four scientists who earned this achievement this year. With expertise in polymer science and gene therapy and diagnostics, Reineke is a world leader in the area of polymer/deoxyribonucleic acid nanostructures for medical applications. The Reineke research group specializes in the synthetic design, chemical characterization, and biological study of novel macromolecules.

Reineke also received the *Macro 2012 Lecture Award* from the American Chemical Society Division on Polymeric Materials: Science and Engineering. In June, Reineke presented a lecture, *Core-Shell Carbohydrate Block Copolymers Designed for the Delivery of Drugs and Nucleic Acids*, at the International Union of Pure and Applied Chemistry World Polymer Congress.

## Ilja Siepmann

**J. Ilja Siepmann** was appointed as *Merck Professor of Chemistry* for a five-year term. This is one of five departmental professorships that recognize and reward the Department of Chemistry's most distinguished faculty. Siepmann is vice chair of the Department of Chemistry and director of graduate studies for chemical physics. He has an outstanding record of research accomplishments and service to the department. Siepmann is one of two Merck professors in the Department of Chemistry. Thomas Hoye is the other Merck professor.

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## Timothy Lodge

**Professor Timothy Lodge** received the *2011-12 Postbaccalaureate, Graduate, and Professional Education Award*. He was one of eight professors from throughout the entire university system to receive this award. This prestigious award recognizes faculty members for excellence in instruction; instructional program development; intellectual distinction; advising and mentoring; and involvement of students in research, scholarship, and professional development.

The Department of Chemistry now has six professors who have been honored with the Postbaccalaureate, Graduate, and Professional Education Award. In addition to Lodge, they include Peter Carr, Christopher Cramer, Thomas Hoye, Lawrence Que Jr., and Ilja Siepmann.

Lodge also received the *2012 Minnesota Award of the Minnesota Section of the American Chemical Society (ACS)*. This award, which is given every three years, honors a section member for outstanding contributions to the chemical sciences. Lodge was honored for his scientific achievements in polymer science research. He has an international reputation as a leading researcher in understanding and controlling nano- and micro-structures that result from combining dissimilar polymer materials in new ways.

Lodge is one of the Department of Chemistry's most distinguished professors and researchers. He is director of the University of Minnesota's Materials Research Science and Engineering Center, which supports interdisciplinary and multidisciplinary materials research and education. He is editor of the ACS journal *Macromolecules,* and the recently launched *ACS Macro Letters.*

Previous winners of this award include current Department of Chemistry professors Wayland Noland and Donald Truhlar, and former faculty Robert Brasted, Paul Gassman, Izaak Kolthoff, and Edward Leete.

## Grants fund important research *continued from page 13*

works, BioAmber, Reluceo and Segetis for state officials, and following those visits up with a public policy roundtable.

- Partnering with the CSTPP and the Minneapolis College of Art and Design (MCAD) to offer a unique outreach program to middle school students. The students met with CSP graduate students to learn about the sustainability loop and polymeric materials, and then worked with MCAD undergraduate designers to design posters, logos, and other materials designed to engage students in green chemistry.

In addition to Hillmyer, faculty participants in the CSP include Thomas Hoye, William Tolman and Theresa Reineke from the Department of Chemistry, Frank Bates and Chris Macosko from the Department of Chemical Engineering and Materials Science, Steve Kelley from the CSTPP, and Geoffrey Coates from Cornell University.

Professor Christy Haynes

### Center for Sustainable Nanotechnology

Chemistry Professor Christy Haynes is bringing her expertise in nanotoxicology to a new multi-institutional center, the Center for Sustainable Nanotechnology (CSN), which has been created with a $1.75 million grant over three years from the National Science Foundation (NSF) Centers for Chemical Innovation (CCI) program.

Center for Sustainable Nanotechnology researchers are investigating how nanoparticles interact with living, ecological systems. Nanoparticles, which are finely divided matter, play important roles in many existing and emerging technologies, including new medical diagnostics and targeted treatments for cancer and other diseases, fuel cells and advanced batteries for hybrid/electric vehicles, and new generation solar cells that have the potential to provide free energy from the sun.

In many applications, nanoparticles are used because only a small amount of material is needed, and they exhibit some unique chemical and physical properties because of their small size, containing anywhere from 10 to 10,000 atoms.

On the downside, relatively little is known about how nanoparticles interact with living organisms or the impact of the unintentional release of nanoparticles from consumer or industrial products on the environment. CSN researchers want to reduce adverse biological and environmental impacts by understanding, predicting, and controlling specific chemical and physical interactions between nanomaterials and biological systems. The Haynes research group will focus specifically on the interaction between nanoparticles and beneficial bacteria, a critical component of the food web.

The CSN brings together the expertise of researchers from six different institutions. In addition to the University of Minnesota, this partnership includes the University of Wisconsin-Madison, the University of Wisconsin-Milwaukee, Northwestern University, the University of Illinois, and the Pacific Northwest National Laboratory. The center's director is Professor Robert Hamers from the University of Wisconsin-Madison.

All graduate students participating in the CSN research will experience a unique collaborative environment with frequent interaction between the various institutions, short stays in collaborative labs, new public outreach opportunities, and explicit training in novel scientific idea generation.

Like the Center for Sustainable Polymers, the Center for Sustainable Nanotechnology may be eligible for even more funding through NSF Centers for Chemical Innovation phase II grants that provide up to $40 million over 10 years.

### Heat Shields for Hypersonic Vehicles

Professor Donald Truhlar is co-principal investigator of a $1.704 million grant from the Air Force Office of Scientific Research, conducting research critical to the development of new heat shields for hypersonic vehicles. The other investigator for the three-year grant is Assistant Professor Thomas Schwartzentruber from the Department of Aerospace Engineering & Mechanics.

"Through this research, we seek to understand the fundamental mechanisms by which energy (heat) is transferred to the surface of hypersonic vehicles," said Truhlar. He is a world leader in the theoretical and computational methods that describe the potentials and dynamics of molecule-to-molecule and molecule-to-surface collisions.

He explained that new concepts for hypersonic Air Force vehicles flying faster than Mach 5 will induce extreme heating conditions requiring new heat shield designs. The air in front of the vehicle gets so hot that air molecules break into atoms. These atoms can diffuse through the boundary layer and exothermically react with the heat shield surface, depositing significant energy to the vehicle. The long-term goal is to understand these gas-surface reactions at the molecular level so that new materials can be tailored to control the energy transfer between a high temperature gas and the heat shield surface.

Professor Donald Truhlar

It has been observed experimentally that oxygen atoms can recombine on silica-based heat shields to form oxygen molecules in electronically excited states, Truhlar said. Such states are long-lived in the gas phase and may serve to lock-up significant energy, which is carried away from the vehicle and thus not transmitted to the surface.

An experimental setup will be designed and definitive experimental evaluation of the production of excited oxygen molecules resulting from oxygen-atom surface recombination will be performed at SRI International's laboratory in Menlo Park, CA. Truhlar's research group will investigate oxygen-silica reactions with electronic excitation. Schwartzentruber's group will provide the modeling link between quantum chemistry and experiment using large-scale stochastic particle simulations of the full experimental environment. The objective is to fully explain this gas-surface reaction phenomenon at the most fundamental level with the potential to impact future heat shield design and capability for high-speed vehicles.

## Awards *continued from page 15*

### William Tolman

**Professor William Tolman**, Department of Chemistry chair, received the *2012 Charles E. Bowers Faculty Teaching Award* from the College of Science & Engineering. This award honors outstanding professors who have demonstrated exceptional interest and commitment to the teaching of students in the college.

Tolman is an award-winning professor and scientist. His contributions to classroom teaching have been extensive. As chair of the department, Tolman works with faculty members on new education initiatives such as the development of the department's first online chemistry course, the transformation of labs into guided-inquiry learning experiences, and infusing green chemistry into courses, laboratories, and research. In his research laboratory, Tolman exposes students and post-doctorates to forefront research in synthetic bioinorganic and polymer chemistry.

He will become editor-in-chief of *Inorganic Chemistry* in January 2013.

### Donald Truhlar

**Regents Professor Donald Truhlar** received the *2012 Faraday Division Chemical Dynamics Award from the Royal Society of Chemistry.* This award honors scientists for their outstanding innovative research on the dynamics of molecules, including spectroscopy, kinetics, or molecular interactions in the gas, liquid, or solid phase. Truhlar is one of the top physical chemists in the world. Some of his outstanding research areas include his work on variational transition state theory; quantum mechanical scattering theory for reaction dynamics; spectroscopy of the transition state; and potential energy surfaces.

Truhlar is one of the University of Minnesota Department of Chemistry's most distinguished professors and researchers. He has written more than 900 journal articles and 80 book chapters, and has edited or co-edited 13 books. He has taught numerous graduate and undergraduate courses, and has mentored 144 graduate students and postdoctoral associates and 70 undergraduate research students. He serves as an associate editor for the *Journal of the American Chemical Society* and editor of *Computer Physics Communications*, and is a member of many national and international scientific organizations.

## Professor Driessen featured in University of Minnesota eBook

Professor Michelle Driessen, general chemistry director, is featured in a University of Minnesota ebook. The ebook combines technology and crowdsourcing to share examples of successful classroom technology use across colleges, disciplines, and campuses.

Driessen's chapter in the ebook is in the "Changing Pedagogies" section where contributors discuss how to move teaching beyond memorization of facts toward interactive coaching and problem solving. She wrote about the role of technology in the transformation of the Department of Chemistry's general chemistry labs.

The free ebook is available at http://purl.umn.edu/125273, or at iTunes U, Google, and Amazon. It is designed for an iPad, Kindle, Nook, or other tablets, but also can be viewed on computers or with web browsers.

# 2011-2012 Donors

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# Donations help attract the best and the brightest

*By Kathy Peters-Martell*

Another great school year is well underway. At the risk of repeating previous reports, our students continue to astound us with their talents, intellect, and enthusiasm. Once again, the College of Science & Engineering incoming undergraduate class had the highest ACT score in the university. And we are recruiting and training the most promising graduate students who are vital to the success of the groundbreaking research going on in the Department of Chemistry. Many of these students are fortunate to be scholarship and fellowship recipients thanks to the donations of our generous alumni and friends.

We are grateful for the many ways our alumni support the Department of Chemistry: providing countless volunteer hours, establishing scholarships and fellowships to support our students, and donating financial resources to enhance the academic program. With your support, we will continue to attract the best and brightest students and retain world-renowned faculty to maintain the excellence of the Department of Chemistry.

When you get a letter or a call from one of our students asking for your support, please consider doing so. Your support is instrumental to the department and our students. If you have questions or need assistance in making a gift to the department, please contact Kathy Peters-Martell, external relations officer for the Department of Chemistry, at kpeters@umn.edu or 612-626-8282.

## Conference room dedication honors legacy of renowned scientists

The Kate and Michael Bárány Conference Room (117/119 Smith Hall) was dedicated in July. The remodeled conference room was a gift to the Department of Chemistry from George Barany, a Distinguished McKnight Professor in the Department of Chemistry, and Francis Barany, a professor of microbiology and immunology at the Weill Cornell Medical Center in New York, and their families. The room honors the legacy of Kate and Michael Bárány (George and Francis' parents): Holocaust survivors; internationally renowned researchers in muscle biochemistry, biophysics, and physiology; tireless advocates for women in science and academia; distinguished educators; and supporters of the University of Minnesota.

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# Tolman named editor-in-chief of Inorganic Chemistry

*Professor William Tolman, chair of the Department of Chemistry, has been named editor-in-chief of* Inorganic Chemistry, *effective January 2013. He has been associate editor of this American Chemical Society publication since 2007.*


Tolman succeeds Professor Richard Eisenberg from the University of Rochester. He has served as the journal's editor since 2001.

The American Chemical Society (ACS) is the leading publisher of peer-reviewed research journals in the chemical and related sciences. It publishes 50 journals, and four of its editor-in-chiefs are professors and leading research scientists at the University of Minnesota.

In addition to Tolman, the other ACS editors-in-chief are:

- Gunda Georg, head of the College of Pharmacy's Department of Medicinal Chemistry and director of the college's Institute of Therapeutics Discovery and Development, who has been editor-in-chief of the *Journal of Medicinal Chemistry* since January 2012;
- Stephen Hecht from the Masonic Cancer Center and the Department of Laboratory Medicine and Pathology in the College of Pharmacy, who will become editor-in-chief of *Chemical Research in Toxicology* in January 2013; and
- Timothy Lodge from the Department of Chemistry and Department of Chemical Engineering and Materials Science, and director of the Materials Research Science and Engineering Center, who has been editor-in-chief of *Macromolecules* since 2001.

As editor-in-chief of *Inorganic Chemistry,* Tolman said that he hopes to continue improving the quality of the journal, boosting the international character of its associate editor ranks, and using social media to broaden the journal's reach.

*Inorganic Chemistry* publishes fundamental studies in all phases of inorganic chemistry. It is the leading journal on inorganic and nuclear chemistry, number one in total citations and impact factor. Its coverage includes experimental and theoretical reports on quantitative studies of structure and thermodynamics, kinetics, mechanisms of inorganic reactions, bioinorganic chemistry, and relevant aspects of organometallic chemistry, solid-state phenomena, and chemical bonding theory. Emphasis is placed on the synthesis, structure, thermodynamics, reactivity, spectroscopy, and bonding properties of significant new and known compounds.

*Inorganic Chemistry* offers both full-length articles and communications of immediate interest as well as invited award addresses, and has earned respect throughout the world for attracting and publishing outstanding research. It also publishes up to three forum issues annually, which consist of a set of thematically linked papers from leading scientists on a multidisciplinary topic of growing interest.