College of Science & Engineering
University of Minnesota

ChemNews

Department of Chemistry Newsletter
Winter 2011

Associate Professor David Blank is one of the creators of Energy and U, a Department of Chemistry outreach program.

Research + Education + Public Policy = Change

Economic development, the environment, public policy, education, and scientific discovery form the foundation of the Center for Sustainable Polymers' mission.

The Center for Sustainable Polymers (CSP) is a unique integration of science, technology, and public policy initiatives aimed at reducing the use of finite fossil fuel reserves for the creation of polymers (plastics).

In addition to advancing cutting-edge polymer research at the University of Minnesota, the center's mission encompasses forming partnerships with industries, teaching students about sustainable materials, and educating and engaging the public.

Sustainable Polymers: To Page 8

Today's scientists reach out to the next generation

Science is fun, interesting, and important—and something that you, too, can do!

Those are the central themes of the Department of Chemistry's outreach programs, which reach thousands of young people and their parents and teachers each year.

Outreach: To Page 6

what's inside

message from the chair

Reflecting on our roles, our past, our future

As the newly named College of Science & Engineering celebrates its 75th anniversary, it is a good time to reflect on the central role that the Department of Chemistry has played in the history of the college and the university.

Throughout that rich and long history, our faculty, staff, and students have pushed the forefront of scientific research, provided in-depth and comprehensive instruction to literally hundreds of thousands of students, and have had an impact on the lives of countless citizens. We are proud of what we have accomplished, and excited about continuing our work as a flagship department in the College of Science & Engineering and the University of Minnesota.

As we begin the new year, it's the perfect time to contemplate how we can change and improve. You can read about some of those changes in the articles featured in this newly designed newsletter. Highlights include the following:

- A new online course for introductory chemistry was successfully implemented last year, and is now undergoing refinement. Such educational initiatives play an important role in college-wide efforts to assess the pros and cons of online learning.
- We introduced the new Center for Sustainable Polymers, which was established with seed funding from the Institute for Renewable Energy and the Environment. In addition to carrying out exciting research aimed at developing new renewable polymers from plants, center participants designed a major display for this year's Minnesota State Fair, which was seen by tens of thousands of visitors.
- New outreach efforts further our commitment to public education, as illustrated by the successful "Energy and U" show seen by thousands of K-12 students.
- A number of recent awards to our faculty recognize their excellence in research and teaching.

Chair William Tolman

Other changes in the department include the retirements of two longtime staff members, Joan Beed and Sheryl Frankel, whose contributions over the years are greatly appreciated. Two new staff positions have been created and filled. Lori-Anne Williams is our new grants coordinator, and is streamlining and overseeing the submission of grant proposals in support of cutting-edge research. Eileen Harvala has joined us as communications coordinator and has taken on the task of rejuvenating our web presence and this newsletter. Do let us know what you think, and keep in touch!

ChemNews
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our alumni—where are they now?

Welcome to "Where are They Now?", which features alumni reflections on their current work and their experiences in the Department of Chemistry. Read more alumni Where are They Now? stories on our website at http://www.chem.umn.edu.

Ed Huttlin, Ph.D.

Current position: Postdoctoral fellow, Harvard Medical School Department of Cell Biology

Education: bachelor's degree in chemistry from the University of Minnesota in 2003; doctorate in biochemistry from the University of Wisconsin, Madison, in 2008

University of Minnesota research: Undergraduate research under the tutelage of Professor Michael Bowser

Work highlights: My research has focused on characterizing the thousands of proteins present in biological systems and understanding the roles that those proteins play in health and disease.

What from your experiences in the Department of Chemistry prepared you for what you currently are doing?:

Many courses, from Professor William Tolman's honors introductory chemistry to Professor George Barany's organic chemistry lectures and Professor Gianluigi Veglia's graduate-level course on enzyme mechanisms, prepared me well for a research career. Without a doubt, the single most important experience was participating in undergraduate research and completing an honors thesis in the lab of Professor Michael Bowser.

"Most importantly, I discovered, firsthand, that scientific research is a creative endeavor and that I, personally, enjoyed the daily challenges it provides."

Early in my undergraduate career, I was interested in the medical applications of biology and chemistry, but was otherwise unsure of my career aspirations. Eventually, I started working in Professor Bowser's lab on a project that blended analytical chemistry with biomedical science. Our goal was to study a nitric oxide molecule, which is produced in the brain and acts as a chemical messenger that participates in key aspects of memory and cognition. Because nitric oxide is a highly reactive gas, it is challenging to measure directly. So, we set out to test a new method for detecting and quantifying nitric oxide using fluorescence. I was fortunate to pursue this as an independent research project, working closely with Professor Bowser, and learning, in the process, how to conduct scientific research from initial planning through writing and defending my work before my thesis committee. Based on this experience, I shifted my sights from medical school to graduate school and have pursued a career in biomedical research. The experience and confidence I gained as an undergraduate researcher provided a strong foundation for my subsequent research endeavors.

Simon K. Shannon, Ph.D.

Simon with his wife, Bridgette, Ph.D., who is also a chemist at Corning, and their son, D'Engelo "DJ". They live in Horseheads, NY.

Current position: Supervisor for Coatings Research, Corning Inc., organic and biochemical technologies research group

Education: doctorate from the University of Minnesota (organic chemistry major) in 2003

University of Minnesota research: As a graduate research assistant (1998-2003), I worked on the development of solid-phase backbone amide linker strategies for the synthesis of lidocaine and procainamide combinatorial libraries (antiarrhythmic and local anesthetic drugs). I developed new quantitative and colorimetric methods for monitoring aldehydes on solid-phase, and designed alternative linker strategies for mild solid-phase synthesis of C-terminal modified peptides, cyclic peptides, and other amide-containing small molecules.

Work highlights: I am responsible for leading a group of scientists and technicians involved in the development of surface chemistry and coatings for life sciences, environmental, and display technologies.

What from your experiences in the Department of Chemistry prepared you for what you currently are doing?:

Through the McNair Scholars Program, I had my first introductions to the chemistry department working in the lab of Professor George Barany. I gained experience with technical writing and presenting. I got initial exposure to teaching. I learned how to build a network that eventually led to acceptance in the University of Minnesota graduate program. As a graduate student in Dr. Barany's group, I was groomed to be an organic chemist. During my time in graduate school, I became a leader; I was exposed to international travel and research conferences; and I built a professional network of research scientists with similar goals and ideals as mine.

"I have used the same training and skills in my previous and current roles."

Send your Where are They Now? submissions to Eileen Harvala at harva015@umn.edu. Read more stories at http://www.chem.umn.edu.

Creation of successful online course not an easy task

Time, energy, creativity, and personal commitment are keys to the success of the Department of Chemistry's only online course.

Transforming a course from the traditional classroom to online is a difficult task; however, General Chemistry Director Michelle Driessen has succeeded in delivering a rigorous, rewarding course to students.

Michelle Driessen works hard to ensure that her students receive the help and information they need to be successful in her online course, which includes expanded office hours where she can work one-on-one or in small groups with her students.

Transformation

The challenges of translating a lecture course to an online version forced Driessen to think creatively about course design, to be intentional about what she wanted to convey in online lectures, and to create or enhance instructional support systems for students.

Online courses offer many benefits to students. They can view the lectures and do the work when and where they want to, allowing for flexible work and study schedules. But there are challenges as well. Students must take the initiative to talk to the professor, whom they don't see in person without making a special effort.

Contrary to some popular opinions, online courses are not cheaper to develop and deliver than traditional classes. Creating and delivering an online course takes as much, if not more, time and energy as a traditional course. Driessen ensures that her course is as rigorous online as it was in the traditional classroom. She also ensures that her students receive the help and information they need to be successful in the course, which includes expanded office hours to encourage students to meet with her in person.

The result of Driessen's efforts is Chem 1015, an introduction to chemistry course, which now is only available online. In its second year, the course had an enrollment of 1,186 students this fall. Another 700 students are expected to take the course in the spring and summer of 2011.

Chem 1015 bridges the gap between high school chemistry and general chemistry courses such as Chemical Principles I & II. When combined with a laboratory component, this introductory chemistry course meets the core physical science requirement. However, a large number of Chem 1015 students take additional chemistry courses.

Similar, but different

The online version of Chem 1015 is similar to the structure of traditional chemistry courses complete with lectures, homework assignments, and exams. Available to students through the University of Minnesota's classroom portal, Web Vista, each online unit also includes lecture videos, practice problems, online homework assignments, practice exams, information that must be assimilated, support links, study group sign-up sheets, exams and answer keys, and frequently asked questions that are updated when necessary. Students can download the video lecture files through iTunesU.

In her videos, which are mini-lectures organized by topic, Driessen talks to, not at, her students. With 12 years of teaching experience, she has come to anticipate students' questions and addresses a lot of those in the videos.

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Online

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Clear communications

Driessen prizes clear communications. She communicates extensively via email, making a personal commitment to respond to her students' individual questions or concerns. In addition, she urges her students to ask questions in person during office hours, to participate in study groups and the class online discussion board, and to seek help in the tutor room.

Like with many freshman-level courses, Driessen said that students sometimes come to her course with unrealistic college expectations. "It doesn't matter if the course is taught online or in a large lecture hall, the students must learn how to study in a college environment and, of course, do the work," she said.

What's next

Courses need to evolve to meet the needs of the students. A next step for Chem 1015 encompasses adding a real-time, video conference component to the course, through which Driessen can interact with students and answer their questions online. She is working with the Department of Chemistry's information technology unit to create these videos.

Questions

While the Department of Chemistry was out-front in creating an online course for the university, there are a lot of questions surrounding online learning. It may not suit the learning styles of all students, may not meet students' expectations, and may not be suitable for all courses.

Currently, an E-Education Task Force is evaluating online learning and what e-technology means for the College of Science & Engineering. Chemistry Professor Ken Leopold serves on that task force, which is looking at a number of e-learning issues such as cost-effectiveness, course quality, and access.

"It can be difficult to discuss chemistry when you're not talking face to face."

—Michelle Driessen, Ph.D.

"We recognized that while online learning works well for some students and for some courses, it is also clear that many of our chemistry courses will not fit an online learning model," said William Tolman, Department of Chemistry chair. "Hands-on laboratories, actually doing experimental chemistry, are a critical aspect of learning chemistry. We cannot lose sight of that."

Access Achievement Award

Michelle Driessen received an Access Achievement Award from the Office of Equity & Diversity's Disability Services for her work on behalf of people with disabilities.

Her work was highlighted at a special recognition ceremony: "When Michelle Driessen and the Department of Chemistry decided to take their Introduction to Chemistry course out of the classroom and deliver it online, they were prepared to do whatever was necessary to make the course accessible to all students. In addition to taking on the labor-intensive investment of videotaping her lectures, Michelle worked closely with Disability Services' Interpreting and Captioning Unit to ensure that each lecture was captioned. That was no small task. However, the end results mean that all students have access to this course."

CyberMULE project gives researchers access to ultrafast spectrometer

Assistant Professor Aaron Massari has been awarded a $470,000 National Science Foundation grant that will provide scientists from throughout the country access to an ultrafast spectrometer.

The project, called the Cyber-Enabled Multi-User Laser Experiment (CyberMULE), encompasses a cyber-enabled instrument that marries modern laser technology with interactive Internet communications. The CyberMULE is a tunable, ultrafast, visible, near-infrared, mid-infrared, pump-probe spectrometer. It will be located in the University of Minnesota's Department of Chemistry, but can be accessed from anywhere in the country through the Internet. Users will have the ability to experiment with their samples and receive data from their remote locations.

This project is designed to primarily serve undergraduate institutions. It is hoped that the CyberMULE will broaden participation for ethnically underrepresented, geographically isolated, or physically disabled users at institutions that do not have access to the advanced equipment.

"The Department of Chemistry at the University of Minnesota prides itself on providing students and researchers, both on and off campus, with access to cutting-edge instrumentation," said Massari. "This new laser facility will bring incredibly sophisticated measurements to the fingertips of nearly any scientist in the nation with an Internet connection and a photochemical question to answer. The design pushes the envelope of 'cyber-enabled experimentation' and will likely serve as a national model for using technology to increase access to user facilities."

More information can be found at http://z.umn.edu/24s.

Today's scientists reach out to the next generation

Outreach: From Page 1

The Department of Chemistry's free outreach program has existed for more than 20 years. Each year, a handful of volunteers—undergraduate and graduate chemistry students—conduct a variety of chemistry demonstrations and discuss chemistry careers in local schools and for a variety of groups. They also participate in special events at the Science Museum of Minnesota, the Minnesota State Fair, the University of Minnesota, and other venues. Last year, the program reached approximately 7,000 young people with more than 45 presentations.

Chemistry concepts

The presentations encompass a number of interesting experiments that illustrate important chemical principles. Several include hands-on experiments designed to actively engage the students, which are facilitated with the help of Joe Franek, Department of Chemistry lecture demonstration director.

The presentations are specifically tailored to students' ages and levels of understanding about chemistry. Materials and advice are provided to teachers. Outreach volunteers also talk about the numerous careers that are possible in chemistry-related fields.

"We want to show that chemistry is fun," said Professor Ken Leopold who directs the program. "We want kids to know, from a very early age, that they, too, can do science, can do chemistry."

There also is a hope that some of the outreach volunteers will be inspired to become educators.

This is what we should be doing, showing our kids that science is fun, that science is interesting, and that science is important."

—Professor Ken Leopold

"The student volunteers really form the backbone of our outreach program," said Leopold. "It is fantastic that they are teaching kids about chemistry." He credits the student coordinators for their work with the program, including Research Assistant Eric Olson who coordinated the program for two years, and this year's coordinator Miranda Hada, an undergraduate student.

Coming to the university

To provide K-12 students and teachers with college-level laboratory experiences and opportunities to meet university faculty members and students, the Department of Chemistry's outreach encompasses inviting them to the university for tours, workshops, and demonstrations. For example, the desired outcome of one general chemistry workshop was to improve the capabilities of teachers on both sides of the high school to college transition to help their students succeed in college chemistry coursework.

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Lecture Demonstration Director Joe Franek creates and facilitates many of the demonstrations used for the Department of Chemistry's outreach initiatives. (Photo courtesy of Patrick O'Leary.)

Explosive Energy and U show ignites students' interest

With an information slide show set to music, and some demonstrations that include loud explosions, bright flashes and flames, one specialized outreach program—Energy and U— is rapidly gaining popularity. Energy and U shows are fun, engaging, educational, and informative—and get young people excited about science.

"We try to emphasize that they, too, could do what we do every day."
—Associate Professor David Blank

Associate Professor David Blank and Professor Marc Hillmyer from the Department of Chemistry, and Professor Frank Bates, head of the Department of Chemical Engineering and Materials Science, started the program in 2006. Joe Franek, the Department of Chemistry's lecture demonstration director, created the demonstrations and is a presenter at many of the shows along with other chemistry department professors.

Last year, these creative scientists put on 10 shows for more than 2,000 elementary through high school-age students and their teachers. This year's goal is to conduct approximately 15 shows, reaching more than 3,000 young people, which includes participating in the College of Science & Engineering's Math & Science Family Fun Fair, and a week-long series of Energy and U shows on the university campus in May 2011.

Energy and U shows focus on how energy can be stored and interconverted in many ways, and that chemical conversions play a key role. "We try to teach the kids that they cannot make or destroy energy, they can just change its form," said Blank.

Students are bused to the university with transportation funding provided by the National Science Foundation Materials Research and Engineering Center (MRSEC), which is led by Chemistry Professor Tim Lodge.

Associate Professor Christy Haynes helps a young scientist with an experiment at an Energy & U show during the College of Science and Engineering's Math & Science Family Fun Fair.

Outreach

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And there's much more . . .

From presentations in school classrooms to microscopy camps and special events such as chemistry days for city programs, many faculty members and chemistry students are involved in education outreach activities. With students of diverse, multicultural backgrounds, especially African-American, Latino, and American Indian, underrepresented in the College of Science & Engineering, outreach to students from diverse backgrounds and from low-income families is intentional. Below are just a few examples of the Department of Chemistry's extensive outreach activities:

- Each spring, the Women in Science & Engineering (WISE) group hosts a "Cool Chemistry" workshop for girls in 7th and 8th grades. The day is chance for girls to explore, hands-on, the wonders of chemistry with women in the chemistry department's graduate program.
- The Minnesota section of the American Chemical Society has one of the most extensive Chemists in the Library programs in the nation. Chemistry Professor Philippe Buhlmann is the principal organizer of monthly visits to community libraries where volunteers from varied chemistry careers and chemistry students help young people and adults with chemistry experiments.
- Alpha Chi Sigma (AXE), a professional chemistry fraternity, conducts demonstrations at many events because it "wants to expose young people, no matter what age, to how cool chemistry can be," said Alisa Wobbema, AXE outreach coordinator.
- Many professors have direct interaction with young people as part of National Science Foundation-funded research.

Alumnus/professor receives outstanding achievement award

The University of Minnesota Board of Regents honored Stanley Bruckenstein with an Outstanding Achievement Award.

The Outstanding Achievement Award honors graduates who have attained unusual distinction in their chosen fields, professions, or public service, and who have demonstrated outstanding achievement and leadership. Bruckenstein was a chemistry professor at the University of Minnesota from 1955 to 1968, and the University of Buffalo from 1968 to 2002; a pioneering researcher in electrochemistry and analytical chemistry; and an outstanding teacher and mentor. He received awards for foundational work on technology used in electronic devices, ranging from cell phones to pacemakers.

Research + Education +

Sustainable Polymers: From Page 1

Launched in May 2009, seed funds for the Center for Sustainable Polymers were provided by the University's Initiative for Renewable Energy & the Environment (IREE) large grant program, which helps launch early-stage, high-potential projects in emerging fields of renewable energy and the environment. Generous industry funding and other support comes from various company affiliates that include Cargill's NatureWorks, LLC, which has been working since 1997 to develop competitive, low-carbon footprint, polymer products made from renewable resources.

Partners

Professor Marc Hillmyer is director of the CSP. He is a professor in the College of Science and Engineering's (CSE) Department of Chemistry, and is a leader in the design, synthesis, and property optimization of polymeric materials.

His CSP colleagues target a range of research and public policy efforts at the university in the area of sustainable polymers science and technology. Principal investigators include Professors Tom Hoye and Bill Tolman from the Department of Chemistry; Professors Frank Bates and Chris Macosko from the CSE's Department of Chemical Engineering and Materials Science; Steve Kelley, director of the Humphrey Institute of Public Affairs' Center for Science, Technology and Public Policy; and Professor Steve Severtson from the College of Food, Agricultural and National Resource Sciences' Department of Bioproducts and Biosystems Engineering.

Focus on renewable resources

CSP's research is focused on the creation of synthetic polymers from renewable and sustainable resources such as soybeans, corn, sugar beets, and pine trees. These new polymers ideally will be commercially viable, produced in an energy-efficient manner, and environmentally friendly, including being non-toxic and compostable. The new polymeric materials also must be competitive with petroleum-derived products, particularly in the areas of strength, elasticity, and heat resistance.

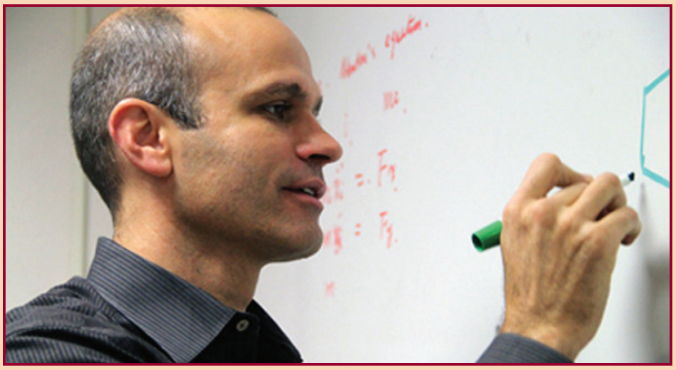
"There is a critical need to reduce our reliance on synthetic chemicals and materials made from crude oil—a non-renewable resource."

—Professor Marc Hillmyer

Critical need

"Our challenge is to develop alternatives from sustainable, renewable resources, meeting our technological needs while preserving Earth's resources," said Hillmyer. "Sustainable polymers—green materials—can be durable, can be degradable, can be used in applications from adhesives to packaging and building materials, and can be produced efficiently and economically with low environmental impact."

Professor Marc Hillmyer has received the prestigious 2011 Carl S. Marvel Creative Polymer Chemistry Award from the American Chemical Society, Division of Polymer Chemistry, Inc. This award recognizes accomplishments and innovations of unusual merit in the field of basic or applied polymer science by individuals younger than 45.



Public Policy = Change

As part of its outreach and education efforts, the Center for Sustainable Polymers worked with the Minnesota Pollution Control Agency to develop an Eco Experience exhibit for this year's state fair. The exhibit was an opportunity for more than 300,000 visitors to learn about sustainable polymers, to see products made from those polymers, to ask questions, and to learn about the center.

Photo by Paul Andre

People could play with molecular models, touch and look at the range of plastic products made from renewable resources such as clothing and fibers, see the life cycle of polymer products made from corn that were composted back into soil again, and learn about polymer research. The display was also intentionally designed to engage young people, illustrating that chemistry is a career with scientists working on relevant solutions to today's issues.

Bill Bushey, a graduate student, Paul Andre from the Minnesota Pollution Control Agency, and Professor Marc Hillmyer, director of the Center for Sustainable Polymers, created the exhibit. Bushey is a second-year Master of Science in Science, Technology, and Environmental Policy candidate and a research assistant for the Center for Science, Technology, and Public Policy at the Humphrey Institute and the Center for Sustainable Polymers.

"By telling people about the applications for sustainable polymers and by making connections with companies, we can tell some good stories to our policy makers, and work to capitalize on resources that can sustain this type of research," said Steve Kelley, director of the Humphrey Institute of Public Affairs' Center for Science, Technology and Public Policy, which is a partner in the CSP.

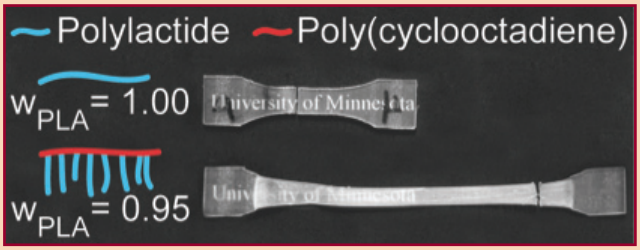
Developing products from renewable resources is an economic development issue as well. Kelley is convinced that new businesses will be created as new uses for crops and other new sources of renewable materials are developed, and the range of applications available is expanded. Those new businesses will have the value-added benefit of also being environmental friendly.

As a public policy student, Bushey said that he realized that scientific research, itself, is not enough. "Some of our other systems have to catch up with the research and technology," he said. "We need to think about needed changes to some of our social institutions and infrastructures. For example, it is great that we are developing packaging that is compostable. But how is it compostable? Where is it compostable? How do we educate and engage the public about what to do and how to do it?"

Bushey said that answering these questions is important and one of the reasons why multi-disciplinary, integrated partnerships such as those forged by the Center for Sustainable Polymers are so important. "We can make science better by integrating different perspectives and disciplines," he said.

Research on renewable, tough, and transparent plastics

Professor Marc Hillmyer



Plastics are indispensable and are used in everything from medical devices to children's toys. However, the majority of plastics are derived from fossil fuels. The finite global supply of those non-renewable resources will eventually necessitate the shift to renewable alternatives. Derived from corn, polylactide (PLA) is a renewable resource and biodegradable polyester produced on a commercial scale that can be found in applications such as disposable packaging. Unfortunately, the inherently brittle behavior of PLA has prevented it from more widespread application. Grayce Theryo, a graduate research assistant in the Hillmyer research group, has focused on utilizing rubber toughening to create more mechanically robust polylactide-based materials. She recently reported in a communication to *Macromolecules* **2010**, *43*, 7394, that creating a polylactide-based graft copolymer results in an increase in tensile ductility. The block copolymer consisted of polylactide arms emanating from a rubbery backbone. The backbone was synthesized first via ring-opening metathesis polymerization to yield a macroinitiator possessing pendant hydroxyl groups. Then, ring-opening transesterification polymerization of lactide was initiated from these hydroxyl groups. Microphase separation of polylactide and rubber in a graft copolymer containing only 5 wt% rubber was confirmed by small-angle x-ray scattering and transmission electron microscopy. The small rubber domain size renders these new composites optically clear which can be beneficial for packaging applications. Tensile testing of the graft copolymer revealed a 14-fold increase in the toughness as compared with the parent homopolymer polylactide. This tough polylactide-based material will open doors to other advanced renewable polymers with mechanical properties that can facilitate more extensive implementation of these next generation plastics.

faculty honors & awards

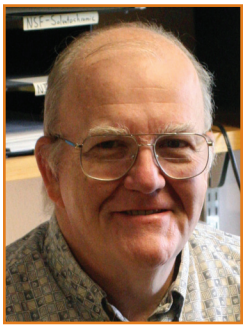
David Blank

Associate Professor **David Blank** received the *2009-2010 Horace T. Morse-University Alumni Award for Outstanding Contributions to Undergraduate Education*. This award honors 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. The honorees' works were publicized to serve as a resource for the whole faculty. Blank was one of six faculty members from across the entire university chosen to receive this award this year.

David Blank

Peter Carr

Professor **Peter Carr** received the *A.J.P. Martin Gold Medal* from the British Chromatographic Society at the International Conference on Column Liquid Chromatography. He also received the *Csaba Horvath Medal* of the Connecticut Chromatography Counsel and the Hungarian Chromatographic Society at the Connecticut Separation Science Council symposium. He was the keynote lecturer at the conference and symposium.


Peter Carr

Christopher Douglas

Assistant Professor **Christopher Douglas** was chosen as a 2010 *"Journal Awardee"* from the editorial boards of Synlett and Synthesis. Awardees are promising young professors at the beginning of their careers, and are awarded free subscriptions to the journals as well as *Synfacts-Highlights in Synthetic Organic Chemistry*. In addition, the Research Corporation for Science Development honored Douglas as a *Cottrell Scholar* for his proposal, "Catalytic Methods in Functionalizing Single Bonds to Carbon." The award honors third-year physical science professors who excel in both teaching and research. It is among the most prestigious fellowships for beginning faculty members in the sciences, and includes an award of $75,000 that Douglas can use for research and teaching. *(Read story on page 12.)*


Christopher Douglas

Michelle Driessen

Michelle Driessen, general chemistry director, received an *Access Achievement Award* from the Office of Equity & Diversity's Disability Services. *(Read story on pages 4 & 5.)*

Jiali Gao

Professor **Jiali Gao** received an *IBM Faculty Award* for his research contributions to the development of novel quantum mechanical methods.


Jiali Gao

Christy Haynes

Associate Professor **Christy Haynes** received the 2010 American Chemical Society Division of Analytical Chemistry *Arthur F. Findeis Award for Achievements by a Young Analytical Scientist*. This award recognizes outstanding contributions to the fields of analytical chemistry by a young analytical scientist. Also, she was selected as an *Alfred P. Sloan Research Fellow*—a competitive award, involving nominations for most of the very best scientists from the United States and Canada. The Alfred P. Sloan Research Fellows program recognizes the achievements of outstanding young scholars in science, mathematics, economics and computer science.


Christy Haynes

Marc Hillmyer

Professor **Marc Hillmyer** has received a number of recent awards. He was named a *Fellow of the American Association for the Advancement of Science*. He was cited for outstanding contributions to the field of biorenewable polymers, particularly, for using block copolymers to control properties and structure on the nanoscale.

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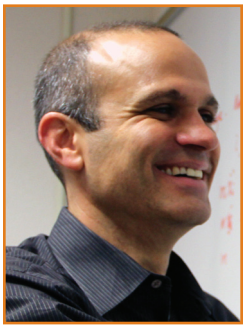
faculty honors & awards


Marc Hillmyer

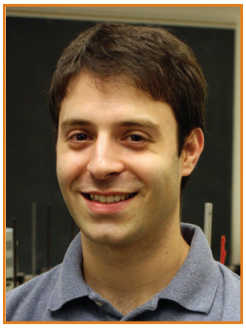
Hillmyer: From Previous Page

He also received the *2011 Carl S. Marvel Creative Polymer Chemistry Award* from the American Chemical Society, Division of Polymer Chemistry, Inc. *(Read stories on pages 8 & 9.)* In addition, Hillmyer received the *2010 Taylor Award for Teaching*. This award is endowed within the College of Science & Engineering in memory of George W. Taylor, a 1934 graduate of the Department of Mechanical Engineering, and is given to tenured or tenure-track faculty members in three categories: teaching, research, and service. It consists of an award citation, and a $2,000 honorarium. Hillmyer also received the University of Minnesota's special mid-career faculty award—the *Distinguished McKnight University Professorship*. This award includes a lifelong title and a grant of $100,000.


Timothy Lodge

Timothy Lodge

Professor **Timothy Lodge** received a *2009 International Award* from the Society of Polymer Science, Japan (SPSJ). Lodge was honored for his excellent contributions to polymer science and to the SPSJ. The SPSJ International Award is the society's highest recognition for scientific achievements and societal contributions to polymer science and technology.


Aaron Massari

Aaron Massari

Assistant Professor **Aaron Massari** was awarded a $470,000 National Science Foundation grant that will provide scientists from throughout the country access to an ultrafast spectrometer (official principal investigator is Chemistry Department Chair William Tolman). *(Read story on page 5.)*


J. Ilja Siepmann

J. Ilja Siepmann

Professor **J. Ilja Siepmann** received a university alumni award for *Outstanding Contributions to Post Baccalaureate, Graduate, and Professional Education*. Recipients are chosen for excellence in instruction; involvement in students' research, scholarship, and professional development; development of instructional programs; and advising and mentoring of students. Siepmann was one of eight faculty members from across the entire university chosen to receive the award this year.


Donald Truhlar

Don Truhlar

Regents Professor **Don Truhlar** was awarded an honorary degree—*Doctor honoris causa*—from the Technical University of Lodz, Poland. He also is part of a $1.5 million *Air Force Office of Scientific Research (AFOSR) Multidisciplinary University Research Initiative (MURI) grant project*, conducting research critical to the development of hypersonic vehicles. *(Read story on page 12.)* In addition, his research group received a *U.S. Department of Energy (DOE) Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Award*, giving it access to a national supercomputer, which is essential for energy research. *(Read story on page 16.)*

Christopher Cramer, Timothy Lodge, and William Tolman

Professors **Christopher Cramer**, **Timothy Lodge**, and **William Tolman** were elected *Fellows for the American Chemical Society for 2010*.

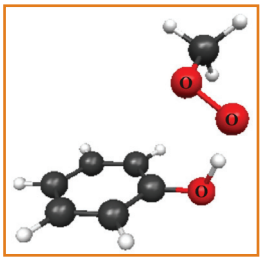

Christopher Cramer


Timothy Lodge


William Tolman

cutting-edge, innovative research

Supercomputer aids with energy research calculations

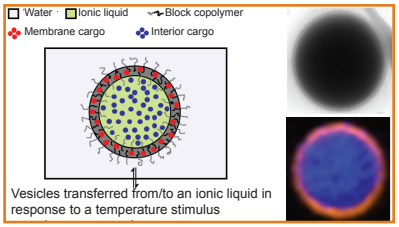


Research Associate Oksana Tishchenko and Regents Professor Donald Truhlar

Regents Professor Donald Truhlar's research group has received a U.S. Department of Energy (DOE) Innovative and Novel Computational Impact on Theory and Experiment (INCITE) award. The INCITE program gives cutting-edge research projects access to supercomputing processor hours. Truhlar's research project has received 15 million supercomputer processor hours at the DOE's Leadership Computer Facility at the Argonne National Laboratory.

Projects receiving INCITE awards utilize complex simulations to accelerate discoveries in ground-breaking technologies. The University of Minnesota researchers will look at potential energy surfaces for simulating complex chemical processes. They will apply multi-reference perturbation theory and multi-configuration quasi-degenerate perturbation theory to study three challenging classes of reactive systems in the gas phase and materials, including charge transfer coupled to magnetic spin state change in metallofullerenes and metal-doped carbon nanotubes; reactions of phenolic antioxidants with free radicals; and radical-radical and radical-molecule association reactions. The project also includes an exploratory study of density functional theory as applied to catalytic reactions at gas-solid and gas-nanoparticle-solid interfaces and to charge transfer at material interfaces. The computer-intensive part of the research consists of electronic structure calculations required for structural characterization and rate constant and dynamics calculations.

Polymersomes with ionic liquid interiors dispersed in water



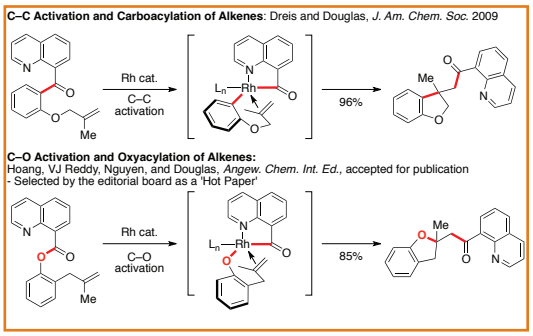
Research Assistant Zhifeng Bai and Professor Timothy P. Lodge

Research Assistant Zhifeng Bai and Professor Timothy P. Lodge recently describes polymersomes with ionic liquid interiors dispersed in water. This vesicle system is of particular interest as a nanocarrier or nanoreactor for reactions, catalysis and separations using ionic liquids. The vesicles are prepared via a simple and spontaneous migration of poly(butadiene-*b*-ethylene oxide) (PB–PEO) block copolymer vesicles from a hydrophobic ionic liquid, 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([EMIM][TFSI]), to water at room temperature. As PB is insoluble in both water and [EMIM][TFSI], and PEO is well-solvated in both media, the vesicles feature a PB membrane with PEO brushes forming both interior and exterior coronas. The PB–PEO vesicles migrate across the liquid-liquid interface with their ionic liquid interiors intact, and form a stabilized aqueous dispersion of the vesicles enclosing microscopic ionic liquid pools. Upon heating, the vesicles can be quantitatively transferred back to [EMIM][TFSI], thus enabling facile recovery. The reversible transport capability of the shuttle system is demonstrated by the use of distinct hydrophobic dyes, which are selectively and simultaneously loaded in the vesicle membrane and interior. Furthermore, the fluorescence of the loaded dyes in the vesicles enables probing of the microenvironment of the vesicular ionic liquid interior through solvatochromism, and direct imaging of the vesicles using laser scanning confocal microscopy (LSCM).

The graphic shows a cartoon of a vesicle in water, filled with ionic liquid, and containing a blue "cargo" dye in the interior and another orange cargo in the membrane. The upper right image is a cryogenic transmission electronic micrograph of a micron-sized ionic-liquid filled vesicle in water; below is a laser scanning confocal microscopy image showing the fluorescence of the two cargoes.

This work is described in "Polymersomes with Ionic Liquid Interiors Dispersed in Water," Z. Bai and T. P. Lodge, *Journal of the American Chemical Society*, **2010**, *132*, 16265-16270.

Catalytic methods for functionalizing single bonds to carbon



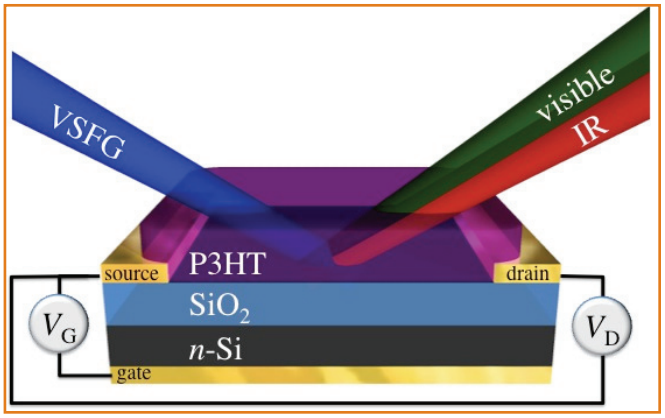
Assistant Professor Christopher Douglas

A major focus in Assistant Professor Christopher Douglas' research laboratory is to discover catalytic methods for functionalizing single bonds to carbon, such as carbon-carbon sigma bonds (C–C bonds) and the C–O bonds of esters. The challenge of activating C–C bonds inspires attempts in the presence of even more reactive functionality, including even the C–H bond. Activated C–O bonds of esters, on the other hand, are highly prone to fragmentation rather than atom economical reactivity. The key problem is not simply convincing a metal catalyst to insert into the bond. Rather, the problem is convincing the catalyst to conduct a useful molecular reorganization with high selectivity.

Douglas' laboratory has demonstrated that C–CN bonds of acylnitriles are readily activated and added across alkenes with high enantioinduction (not shown). The new method is a viable strategy for constructing indole alkaloids, which have been identified as privileged structures in drug discovery. Rhodium catalysts can activate the C–C bond adjacent to a ketone, and the acyl C–O bond of esters, in the presence of an appropriate chelating group such as a quinoline (see graphic). Highly selective carboacylation or oxyacylation, respectively, of alkenes can be achieved.

Spectroscopic techniques that only produce signals from sample interfaces

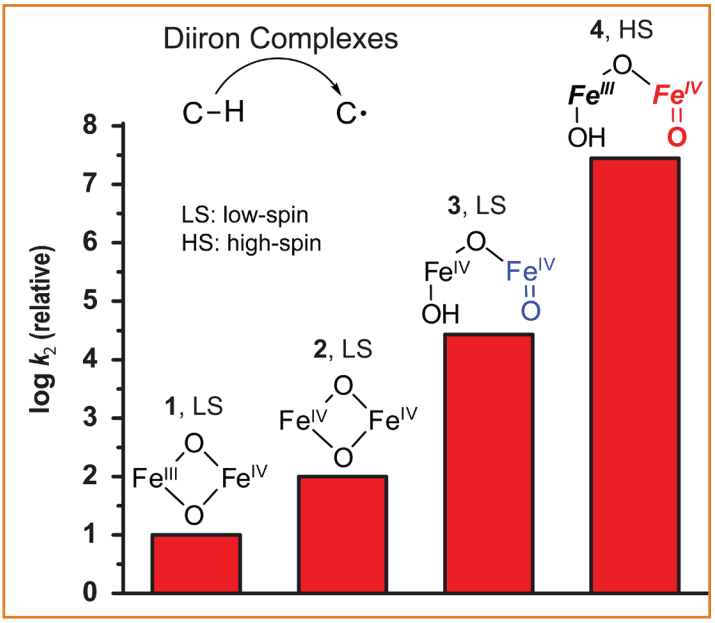
Assistant Professor Aaron Massari



Field-effect transistors (FETs) are at the heart of every digital electronic device, from laptops to checkout scanners. Typically, the active materials in these transistors are inorganic semiconductors such as silicon. There is a strong drive to replace these heavy, expensive materials with cheap, lightweight, carbon-based semiconductors. During operation of these organic FETs, or oFETs, a molecularly thin layer of the active material is electrochemically transformed into a conductor, presumably accompanied by structural adjustments following the electron transfer process. The mobility of electrical charges through these devices is then defined by the molecular structures in this thin interfacial slab of the organic semiconductor. Measuring the chemical changes in this crucial region is particularly challenging since it is buried beneath 50 to 100 molecular thicknesses of inactive material. This is akin to trying to measure the behavior of the bottom most centimeter of water in the Mississippi river from a bridge in Minneapolis without disturbing the river's flow. Fortunately, there are spectroscopic techniques such as vibrational sum frequency generation (VSFG) that only produce signals from sample interfaces. Assistant Professor Aaron Massari's research group has been utilizing this approach to measure the infrared spectra of the molecules that reside at the buried interface in oFETs in order to understand how the interfacial structure differs from the bulk material, and how it changes in response to device switching. Recent work from this project was published in the *Journal of Physical Chemistry C* **2010**, *114*, 17629. VSFG spectroscopy was used to probe the polymer-silica interface of poly(3-hexylthiophene) oFETs in-situ during device operation. The VSFG spectra from the buried interface exhibited dramatic changes upon switching. Notably, the spectral changes were observed when the oFET was activated with both positive and negative voltages, despite unipolar current-voltage responses. This supports a model in which electrons accumulate at the buried interface but are quickly trapped and immobile.

Million-fold activation of an $[Fe_2(\mu\text{-}O)_2]$ diamond core to cleave C–H bonds

Research Associate Gen-Qiang Xue and Regents Professor Lawrence Que Jr.



The hydroxylation of methane to methanol in nature is carried out by the nonheme diiron enzyme methane monooxygenase (MMO) found in bacteria called methanotrophs. The fact that this challenging transformation occurs under mild conditions has elicited strong interest in understanding the nature of the oxidant. The nonheme diiron center of MMO activates dioxygen to generate a powerful oxidant called Q, which is postulated to possess a high-valent $[Fe^{IV}_2(\mu\text{-}O)_2]$ diamond core (**2**). The synthesis of biomimetic complexes with such diamond cores and the characterization of their C–H bond cleavage reactivity could enhance understanding of the MMO mechanism. Toward this end, Research Associate Gen-Qiang Xue in the laboratory of Professor Lawrence Que Jr. has been investigating the chemistry of a crystallographically characterized complex that has an $[Fe^{III}Fe^{IV}(\mu\text{-}O)_2]$ diamond core (**1**). As this complex is stable enough to be crystallized, it is not surprising that it is fairly sluggish in reacting with C–H bonds and can cleave only C–H bonds of less than 80 kcal/mol in strength (compared to 104 kcal/mol for methane).

In a recent paper published in *Nature Chemistry* **2009**, *2:* 400, Xue and coworkers reported the conversion of this synthetic complex into a million-fold more reactive species by treatment with hydroxide. Spectroscopic studies showed that the diamond core complex was transformed into a new species with an open $[HO\text{–}Fe^{III}\text{–}O\text{–}Fe^{IV}\text{=}O]$ core (**4**). This activity enhancement results from two factors: the formation of a terminal oxoiron(IV) moiety (similar to that of **3**) and the conversion of the iron(IV) center from low-spin (S = 1) to high-spin (S = 2). Both factors each enhance C–H bond cleavage reactivity by a thousand-fold. These results suggest that a similar core isomerization might occur in the active site of methane monooxygenase for the cleavage of the methane C–H bond.

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While the start of a new year is traditionally a time to set goals and aspirations for the days ahead, it is also a time to reflect on all that was accomplished in the previous year and to express our gratitude for the many ways our alumni, faculty, and friends support the Department of Chemistry with donations of time, talents, and financial resources. This generosity continues to enhance our rigorous academic program and support our amazing students, faculty, and the research activities. Your support is integral to the continued tradition of excellence in the Department of Chemistry, and we thank you.

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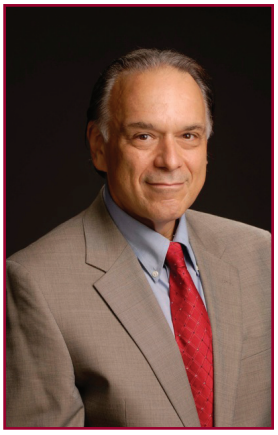

Paul F. Barbara, a prominent scientist, teacher, and former Department of Chemistry faculty member, died on Sunday, October 31, due to complications following a cardiac arrest.

He was a member of the University of Minnesota's Department of Chemistry for 18 years, from 1980 to 1998, before accepting a position in the Department of Chemistry and Biochemistry at the University of Texas at Austin.

He received many awards throughout his career, including being named the 3M-Alumni Distinguished Professor of Chemistry while at the University of Minnesota. During his career, he also was awarded a Presidential Young Investigator Award, and the E. Bright Wilson Award in Spectroscopy. In 2006, he was elected to the prestigious National Academy of Sciences.

"Paul was a scientific leader, friend, mentor, and congenial colleague," said William Tolman, Department of Chemistry chair. "We will miss him."

Please read more about Paul Barbara's accomplishments and legacy at http://z.umn.edu/248.

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in the news

Research critical to development of hypersonic vehicles

Regents Professor Donald Truhlar is part of a $1.5 million Air Force Office of Scientific Research (AFOSR) Multidisciplinary University Research Initiative (MURI) grant project, conducting research critical to the development of hypersonic vehicles.

The Air Force plans to develop hypersonic vehicles that will be in the atmosphere for extended period of times. Those vehicles will be exposed to high temperature interactions between gases and the vehicle surfaces, resulting in the need for advanced thermal protection systems.

A world leader in the theoretical and computational methods that describe the potentials and dynamics of molecule-to-molecule and molecule-to-surface collisions, Truhlar will bring his expertise in quantum chemistry and reaction dynamics to the research team. He will use high-level modeling—quantum mechanical electronic structure calculations—to look at hypersonic flow problems involving the vast number of molecular-scale interactions between gases and vehicle surfaces. He will apply recently developed, highly successful, density functionals and wave function theory to develop interaction potentials.

Truhlar also will be working on the development of force fields that can be used to predict energy transfer cross sections and chemical reaction rates during gas-phase and gas-surface collisions in simulations of shock layers around the vehicles.

Sensor technology invention could aid the environment

Associate Professor Philippe Buhlmann has invented a sensor that detects and measures ions found in chemical solutions. Buhlmann is a leading researcher on fluorous membrane technology.

Buhlmann's fluorous ion selective electrode (ISE) sensor membrane is longer lasting, more durable, and has improved selectivity and less interference than other ISE sensor membranes. The sensor could prevent toxic by-products of mining and other industries from ending up in the environment through the waste stream.

The sensor technology has been licensed by the University of Minnesota to United Science for possible initial use by mining companies. United Science is headed by Jon Thompson who earned his doctorate in chemistry at the university.

For additional information, read the university's news release at http://z.umn.edu/26l.