

COLLEGE OF
Science & Engineering

UNIVERSITY OF MINNESOTA

CHEMnews

DEPARTMENT OF CHEMISTRY NEWSLETTER

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Repertoire of modern innovative teaching methods engages students in learning



Professor Michelle Driessen

Online courses, hybrid flipped classrooms, problem-based and guided-inquiry laboratories are altering how faculty teach, and students learn.

The times they are a changing, and when it comes to teaching undergraduate students, the Department of Chemistry is leading the way with innovative teaching methods in its classrooms and laboratories.

Online courses, hybrid or flipped classrooms that combine online learning with in-class focused, interactive learning activities, and problem-based and guided-inquiry laboratories are part of the re-imagined teaching repertoire in the Department of Chemistry. The department is at

the forefront of the latest modern and innovative teaching pedagogy for its large-enrollment general chemistry and organic chemistry courses. It is also a pioneer with its uniquely designed analytical curriculum and laboratory and its advanced chemical biology laboratory.

Leading this innovation are professors David Blank, director of Undergraduate Studies, Michelle Driessen, general chemistry director, Nicholas Frost, analytical laboratory director, and Jane Wissinger, organic chemistry director.

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CHEMnews

DECEMBER 2015

DEPARTMENT OF CHEMISTRY CHAIR
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The Department of Chemistry is dedicated to excellence in education, research, and public service. We strive towards these goals through world-class teaching in the classroom and laboratory, research aimed at solving some of society's most important human health, energy, and environmental problems, and embracing diversity of communities and ideas to benefit Minnesota, the nation, and the world.

This publication is available in alternative formats upon request. Direct requests to Eileen Harvala at 612-624-0831 or harva015@umn.edu.

The University of Minnesota is an equal opportunity educator and employer. The University's mission, carried out on multiple campuses and throughout the state, is threefold: research and discovery, teaching and learning, and outreach and public service.

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Innovative teaching, outstanding researchers, key advisers



Chair William Tolman

Our beautiful Minnesota fall is the perfect backdrop to inspire the teaching and learning taking place in our classrooms and laboratories.

I marvel at the high levels of activity from our students, researchers,

and faculty. For me, what's most exciting is seeing students huddled over their laptops or textbooks, speaking the language of chemistry. That tangible sign of learning is priceless.

Driving that learning is innovative teaching by our faculty and teaching assistants. They are using a full palette of tools to make chemistry come alive for students at all levels, and from all over the university. These extraordinary efforts are highlighted in this issue of our annual newsletter, with particular emphasis on new developments in our undergraduate program. I'm proud of our faculty's deep commitment to finding new ways to grab the attention of the iPhone generation and instill knowledge and excitement about chemistry. This is especially important because too many people in our society seem to mistrust science and the central role it must play in addressing our most challenging problems.

Our faculty members continue to be recognized for their teaching excellence. With the designation of professors Philippe Buhlmann and Lee Penn as winners of the university's two top awards in 2015, we now have 15 members in the Academy of Distinguished Teachers, the largest number and percentage for any department at the university.

Despite these successes, we need modern laboratories to best train students in the practical art of chemistry with spaces for experimentation, and spaces where students can discuss, collaborate, and present what they have learned. We aim

to tackle this problem head-on with a major building project included in the University of Minnesota's six-year capital plan, beginning with a new teaching laboratory facility and then leading to a subsequent renovation of the 100-year-old Smith Hall. These projects will significantly boost our ability to implement innovative teaching methods as well as enable us to grow our faculty and significantly enhance our research efforts.

As we begin planning for this daunting undertaking, we are seeking help from a newly constituted Chemistry External Advisory Board (CEAB) composed of outstanding alumni and industry leaders (see story on page 11). CEAB members are tasked with providing wide-ranging advice, acting as ambassadors for the department in their organizations and beyond, and helping with philanthropic efforts. Discussions at our two meetings this year have already set the stage for successful efforts to improve the stature of the department, enhance our teaching effectiveness, and push research to an even higher level.

Speaking of research, quite a few recent exciting developments have been highlighted on our dynamic website (www.chem.umn.edu). In this newsletter, we feature the work of Regents Professor Donald Truhlar and Professor Theresa Reineke. They have made important inroads in changing the way we think about key problems in theoretical and polymer/biological chemistry, respectively.

The list of awards to our faculty continues to grow, and I'm proud of the extraordinary science that all of our faculty do. Enjoy reading about what's happening in the department, keep in touch, and think about supporting us in any way you can!

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www.chem.umn.edu



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Blindness does not stop theoretical computational chemist from achieving her goals

With tenacity and courage, Mona Minkara turns what others may consider 'impossible' into the possible.

Even when she was a small child, she always wanted to be a scientist. She was curious about how the world worked. Her inspiration came from Bill Nye the Science Guy, the Magic School Bus, and Sherlock Holmes. She was intrigued that the detective could see footprints and determine who made them.

For Mona Minkara, a post-doctoral associate working with Chemistry Professor J. Ilja Siepmann, nothing was impossible for those scientists, and nothing was impossible for her. With tenacity, courage, and stubborn resistance to “you can’t do that,” from an early age, Mona has turned the impossible into the possible. It isn’t always easy. Mona is legally blind, diagnosed at the age of 7 with a genetic, degenerative eye disease. Her current vision is limited to a small amount on the periphery of her left eye, and the ability to distinguish light from dark. Her younger sister is also blind.

At the University of Minnesota, in addition to her support from Professor Siepmann, she is aided by six accessibility assistants who are her eyes, and read information and documents to her. She has computer and phone equipment that talks to her, and special magnifying instruments. She has also memorized her computer keyboard.

With strong encouragement from her parents, Mona has learned to forge her own way in the scientific community, figuring many things out for herself and for others along the way. She was in special education throughout her K-12th grade education in her hometown of Hingham, MA. But she loved math and science and, in her sophomore year, insisted that she be allowed to take Advanced Placement biology despite the teacher’s objections. She

earned one of the highest grades in the class, and received an apology from the teacher who became an invaluable mentor and guide.

Mona majored in chemistry and Middle Eastern studies at Wellesley College. “I originally thought that I might be a doctor,” she said. “I took a lot of classes based on interest and changed my major many times. But then I took a quantum mechanics class taught by a great teacher, and that helped me focus on computational chemistry.”

She conducted research throughout her undergraduate program, including four summers conducting computational research as part of the National Science Foundation’s Research for Undergraduates program. While at Wellesley, she received a one-year research grant from the Howard Hughes Medical Institute. This grant enabled her to work with Professor Mala Radhakrishnan after graduation. She spent that year researching properties of affinity and specificity using canonical enzyme/inhibitor complex of trypsin and bovine pancreatic trypsin inhibitor.

As she did in high school, Mona advocated for herself, teaching others, including the university, about what she needed. For example, she needed readers, called accessibility assistants, who help her read text, and specialized equipment.

“I had to fight a lot because people did not understand what I needed,” she said, “but overall the experience was amazing.” Professor Radhakrishnan, her adviser, invested time and effort into working with Mona, including the publishing of her first two papers as an undergraduate. A network of students helped her through, and one reader in particular, Pam



Mona Minkara, Ph.D.

Davis, became a deeply cherished personal friend.

When applying to graduate school, Mona sought a place that wanted her, and with a disabilities office committed to offering her help and support. She found that at the University of Florida, Gainesville, receiving assistance from the state of Florida and her coordinator Mary Anne Hastings. Mona worked with Professor Kenneth M. Merz Jr., and her graduate-school mentor for five years was post-doctorate Mike Weaver, Ph.D. Mona studied *Helicobacter pylori* urease using molecular dynamics, with a goal of identifying novel inhibitors for the enzyme.

After graduate school, Mona was faced with a choice—a hard one—accept a post-doctoral position at Northeastern University in Boston, which is near her hometown of Hingham, and go home to her beloved family, or accept Professor Siepmann’s invitation to join his research team at the University of Minnesota.

continued on page 4

Theoretical computational chemist *continued from page 3*

Siepmann leads a statistical mechanics research group specializing in particle-based computer simulation. In particular, he is interested in the development of efficient Monte Carlo algorithms and accurate force fields, and their application to the understanding of existing and the discovery of novel materials and separations process. Siepmann is also director of the Department of Energy-funded Nanoporous Materials Genome Center (NMGC), focusing on discovering and exploring microporous and mesoporous materials, which are important to energy technologies.

The goals of Mona's research projects, which are supported through National Science Foundation grants, are to understand and predict phase behavior and spatial distribution of complex molecules in microheterogeneous environments.

"Ilja convinced me to come," said Mona. "He saw my research, and believed that I could do great things at the University of Minnesota. I saw this as an opportunity to learn new things, do some different research, and study polymers."

"During her Ph.D. research, Mona excelled in extracting mechanistic information for complex biochemical systems from molecular

simulations," said Siepmann. "This knowledge and her special viewpoint toward quantifying structural information will prove very useful for our research projects," he said.

Having Mona come to the University of Minnesota has been a learning experience for everyone involved, particularly, Annie Bartels, managing director for the NMGC.

"Mona already had a good sense of the human and material resources she would require because she already developed and honed these methods during graduate school," said Annie. "My efforts were largely figuring out how to make what she needed a reality within the University of Minnesota infrastructure in coordination with the appropriate individuals and offices such as the Disability Resource Center (DRC)."

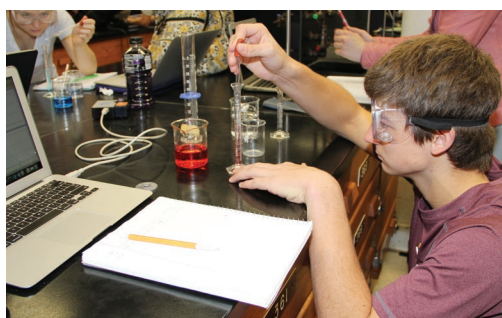
While this all sounds relatively simple, said Bartels, the DRC has never worked with a chemist who is blind, and there was little precedent. There were many meetings and conversations and there were a lot of decisions and levels of approval to navigate. "Overall, it was a lot of organization, coordination, advocating on Mona's behalf, and ensuring follow-through," she said. Mona said that she is deeply appreciative and thankful for all of the help and support from Bartels and the DRC.

Mona said that she loves Minnesota, loves the research that she will be involved, and appreciates Professor Siepmann and Annie for their invaluable support. "I am a challenge," she said. "Not everyone wants to take that on. It takes a visionary like Ilja to work with someone like me."

Blindness has shaped her personality, Mona said. But it does not define her as a person, as a scientist. Her parents, particularly, her "amazing" mother, taught her from an early age that she could do whatever she wanted. If there were challenges, she needed to figure out a way to overcome them.

Mona plans to conduct research at the University of Minnesota for two to three years, working toward the goal of a faculty position in academia. Her hobbies include a variety of physical activities such as horseback riding, zip lining, whitewater rafting, tandem biking, rock climbing and martial arts. Her other hobbies include knitting, hand drumming, and listening to music and audio books. She also composes short stories and posts them on her blog at www.banana-days.tumblr.com. You can learn about Mona on her website at <http://monaminkara.weebly.com/>.

Innovative teaching methods *continued from page 1*



Christopher Greve, who is enrolled in the general chemistry laboratory, uses UV/Vis spectroscopy to identify artificial colors present in a consumer beverage, and then recreates the color profile using food dyes provided in the laboratory.

Professor Erin Carlson created the department's advanced chemical biology laboratory—a first of its kind for the Department of Chemistry.

In general and organic chemistry, the department is one of a few, large-enrollment chemistry programs nationwide that uses problem-based and guided-inquiry approaches in its laboratories. These approaches are designed to help students develop their critical-thinking and problem-solving skills, to teach them how to work effectively in teams, and to encourage them to become comfortable with adapting-on-the-fly in the lab.

"We are making changes in our teaching pedagogy so our students are prepared for research in industry and academia, and teaching. We are hearing from industry leaders that they expect students to work collaboratively in teams, be critical thinkers, and be innovative problem-solvers," said Blank.

Problem-Based Laboratories

Driessen has worked hard to move her general chemistry laboratories away from the traditional laboratory model of "cookbook" or "recipe" experimentation. No longer are students given carefully prescribed experimental proce-

dures to follow step-by-step. Instead, they are presented with one-paragraph problems and asked to design and carry out experiments to solve those chemical questions. Working in teams, the students delve into practical aspects of the experiment such as: What questions are they trying to answer? What observations might provide answers? What experiments might help? If the experiments don't work, what might they do next?

In a typical lab, students perform experiments and trouble-shoot any problems they encounter, give oral reports and discuss what they learned, summarize their progress, and plan for their next lab session. Teaching assistants coach the student teams through the problem-solving process.

Goals for students include experience in experimental design, and thorough, practical knowledge of basic laboratory skills. Project-based labs also engage students in teamwork, foster creativity in science, and emphasize strong written and oral communication. Grading is based on group and individual work, plans, summaries and presentations, lab notebook pages, peer reviews, and formal reports. These laboratory courses are also completely digital, with the lab manual embedded into electronic laboratory notebooks.

"Students learn basic lab skills while practicing and discussing real science," said Driessen.

Guided-Inquiry Laboratories



Professor Jane Wissinger

In Wissinger's organic laboratories, a guided-inquiry approach means that every experiment begins with a question that needs to be addressed. Teaching assistants lead the students in pre- and post-laboratory student-driven

discussions that are designed to engage the students and build critical-thinking skills.

The department's organic chemistry guided-inquiry laboratories are also focused on

green chemistry. Wissinger is a national leader in creating and implementing green chemistry experiments, which exemplify modern strategies used by academia and industry to develop chemical syntheses and processes that are "benign by design" and address issues of sustainability. Students are trained in the principles of green chemistry and explore topics such as the use of renewable materials, solvent-less reactions, and catalysts. The green emphasis also has cut in half the amount of chemical waste produced in the labs.

For Wissinger this is an exciting time for students to be interested in chemistry where "there is both challenge and opportunity to solve society's most pressing environmental and sustainability problems through green chemistry innovations." Additionally, she hopes that "all of the students enrolled in this course carry with them a heightened awareness of the relevance of chemistry in their lives."

Flipped Classrooms

Driessen developed an online introductory chemistry course about six years ago. She has now used that expertise to develop two hybrid general chemistry courses. Her hybrid model, in some ways a flipped classroom model, is unique due to the reduced seat time for students and what those students do during class time. Rather than meeting for 150 minutes in class each week, the students see Driessen for one 75-minute problem-solving session.

Outside of class, students watch videos and

take notes, work on sample problems, do online homework problems, and take advantage of Driessen's office hours. Students meet once a week for face-to-face problem-solving activities. Working in groups of nine at their tables, students spend class time focusing on those activities, respond to selected questions with electronic clickers or color cards, sketch their work on white boards, and view chemical demonstrations. Driessen checks in with the class several times to make sure groups are working through the activities and understanding the concepts.

This is not the department's first flipped classroom. Based on his experience teaching a Massive Open Online Course, Professor Christopher Cramer developed a flipped classroom for the department's computational chemistry course.

Technology & Space Needs

These modern models of teaching in classrooms and laboratories require different spaces. Active-learning pedagogies work best using round tables, laptop connections, and projection equipment. That kind of space is available in Bruininks Hall.

Modern laboratories not only need space for experiments, but also spaces where students can discuss their experiments, collaborate in groups, and give presentations. Those spaces currently don't exist in the Kolthoff Hall and Smith Hall laboratories, thus, driving the current effort to build a new teaching laboratory building.

"We have multi-disciplinary experiences for students that are not found anywhere else. We are pushing forward with innovative learning opportunities for students, and our undergraduates are benefitting from those experiences."

— Professor Erin Carlson

Department designs unique laboratory curriculums focusing on important research

Analytical lab, chemical biology lab, and polymer lab courses engage students in real-world health, environmental, and energy issues, and prepare them for research realities.

The Department of Chemistry has a number of unique laboratory experiences for its chemistry majors and graduate students, including its analytical lab, chemical biology lab, and polymer lab.



Samantha Johnson and Courtney Matthews work on an analytical experiment determining the fluoride concentration in wastewater.

Analytical Laboratory

For the department's analytical chemistry program, Professor Nicholas Frost leads students in problem-based laboratories focused on real-world applications. Students design all of their own analytical methods to answer the big picture analytical problems that are given to them over the course of two lab periods. Through being able to put their own plans and ideas into action, students are learning how to properly design an analytical method. They can see firsthand what happens if part of their method wasn't designed well. During their second lab period, students then have an opportunity to reconsider their plan and learn from what they discovered in their first lab period. They also learn how to perform appropriate statistical analysis of experimental data to reach big picture conclusions, and how to think critically about their methods based on their findings.

Students focus on real-world issues and questions such as the analysis and treatment of wastewater in the manufacturing of semiconductors; the analysis of pharmaceutical components in a new-to-market nasal spray; and the analysis of caffeine and theobromine in the manufacturing of dark chocolate.

"Students, in general, are initially unsure of how to approach a lab where they have so much freedom," said Frost. "But, as the semester progresses, it is clear that students are growing as chemists to a much greater extent than in the past with the old procedure-based curriculum."

Chemical Biology Laboratory

Professor Erin Carlson, who has expertise in organic synthesis, mass spectrometry and other methods critical for mapping biological interactions, was asked to develop a chemical biology laboratory course—the first of its kind for the Department of Chemistry. With few examples of such courses in the nation, she spent about nine months putting together the curriculum from scratch when she first joined the faculty at the University of Minnesota less than two years ago. The goal of the course is to expose students to the application of modern chemical concepts and techniques to biological problems.

One of the components of the chemical biology lab is the study of a protein that is responsible for the resistance of many pathogens to current antibiotics. Students test different drugs on this protein to see if they might be effective for the treatment of resistant organisms. Students also learn about protein purification



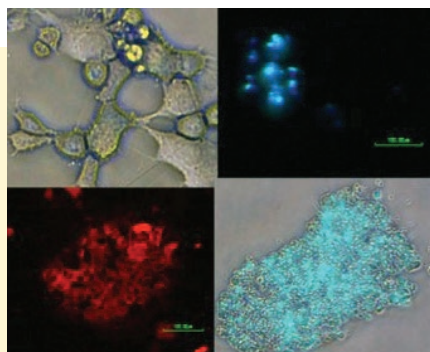
Teaching Assistant Erin Duffy helps Henok Yared and Yuting Qiu with their analytical laboratory experiment trying to determine the concentration of citric acid in soda.

and crystallization, which is critical for understanding the structure of a protein and, thus, potentially designing new therapeutic agents. Course participants have the opportunity to use cutting edge instrumentation, including a microplate reader, a high performance liquid chromatography apparatus, and a fluorescence microscope, which enables them to see the protein crystals that they grow and cancer cells that they examine in another experiment.

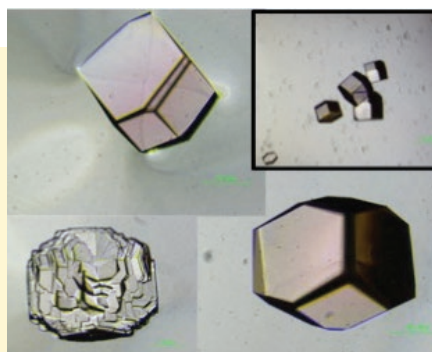
Teaching assistants Lee Godsey, Elyse Krautkramer, Matt Styles, and Peter Ycas had a major role in development of the experiments. They helped Carlson research and test protocols to ensure that those experiments worked well and illustrated the important concepts being studied.



Elena Werst and Dan Nguyen use gel electrophoresis to look at two different proteins.



Cancer cell images



Protein crystal images

"The main goal is to expose students to modern biologically-oriented research that wasn't previously in our curriculum," said Carlson. Another goal is for students to understand how chemistry and biology are related, and why that interdisciplinary focus is important to the study of human biology and therapeutic development.

The course was instantly popular, exceeding capacity for three sections when it was first offered last spring. Even with the addition of another section, there was still a waiting list.

"This is a great opportunity for our students, and it is pretty unique," said Carlson. The enrollment interest illustrates that it was wanted and needed.

Like many faculty members in the Department of Chemistry, Carlson strongly believes that interdisciplinary science is important, and it is critical for students interested in research to be exposed to the fields that bridge the traditional scientific disciplines.

"We have multi-disciplinary experiences for students that are not found anywhere else," she said. "We are pushing forward with innovative learning opportunities for students, and our undergraduates are benefitting from those experiences."

Polymer Laboratory

The Department of Chemistry has had a polymer laboratory for a number of years, with students taking the polymer synthesis course the semester before. Enrollment demand for the laboratory has increased significantly the past

few years. Professors Marc Hillmyer, Theresa Reineke, and T. Andrew Taton have refined the curriculum for the laboratory, and Reineke has taught the lab for the past three years.

The purpose of the polymer lab is to teach graduate students how to synthesize and characterize numerous polymeric materials that are currently used and applied in many of our everyday products. They learn why polymers impart special physical and chemical properties and perform a variety of polymerization routes/mechanisms. For example, the students learn free radical, anionic, reversible addition fragmentation chain transfer polymerization (RAFT), ring opening polymerization, microemulsion polymerization, and thermosetting. The students also learn how to characterize the chemical structure, molecular weight, assembly, thermal, mechanical, optical, and shape memory properties.

The Department of Chemistry has a world-renowned polymer program, and teaching this polymer lab further strengthens the curricula at the undergraduate level. This course is not common in a chemistry department curriculum.

"The polymer industry is one of the largest employers of chemistry graduates," said Reineke. "We teach the students most of the commonly applied polymerization routes and characterization techniques that are used both in industry and for research purposes. We are, thus, preparing our graduates for direct employment in the large range of industries impacted by polymer chemistry."

Alumnus James Phillips honored for mentoring excellence

Alumnus James Phillips, a professor of chemistry at the University of Wisconsin-Eau Claire, received his university's Excellence in Mentoring Research, Scholarship and



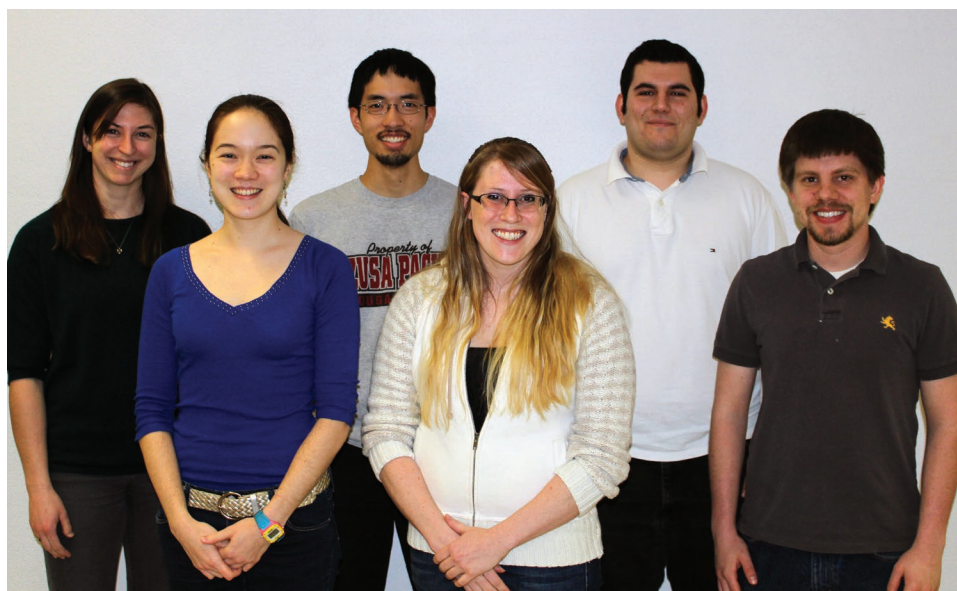
Creative Activity Award. This is his campus' premier award given to faculty for their skill and dedication in mentoring student scholarly projects.

Professor Phillips has mentored 30 students and had 36 student co-authors on peer-reviewed papers since coming to UW-Eau Claire in 1998. Two facets of his work were particularly cited by the reviewers: his focus on intensive development of student writing and his willingness to provide opportunities to a broader range of students by reaching out to those who appear to be less academically prepared or successful.

Phillips earned his doctorate in 1996, under the tutelage of Professor Kenneth Leopold. He has been a professor at UW-Eau Claire since 1990.

Joint Safety Team continues its work on improving the culture of safety

CARE—Compliance, Awareness, Resources, Education—are the foundation of the work of student- and post-doctorate-led safety initiative.



Members of the Joint Safety Team leaders are, from left, Haley Phillips, public relations chair; Alyssa McKenna, analysis and compliance chair; Clifford Gee, finance officer; Melissa Baudhuin, president; Michail Vlysidis, technology officer; and Phillip Goff, education and resource chair.

There's no doubt that safety is an important part of our department's culture. Walk the hallways and you see large safety posters on a variety of different topics on the walls. Attend a seminar, and you see and hear a safety moment. Walk into a laboratory space and, whether a visitor or a researcher, wearing proper safety gear is mandatory.

Leading the charge is the Joint Safety Team (JST). Since its beginning three years ago, the JST is lead by graduate student or post-doctorate Laboratory Safety Officers (LSOs) in the departments of Chemistry and Chemical Engineering & Materials Science (CEMS). Melissa Baudhuin is the current JST president, following Katie Hurley and Kathryn McGarry.

The Joint Safety Team began through a unique partnership with Dow Chemical Company. Dow shared its best-in-class laboratory safety practices, examples, advice, and resources with University of Minnesota students and post-doctorates. The JST initiated a safety campaign,

called Safety Starts with U!, which 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;

Education: Improve safety training and ongoing education for laboratory safety officers and researchers.

This safety campaign is an important guide for the continuing and evolving work of the JST. For example, some industry leaders have clearly indicated that they are looking for researchers

who are knowledgeable and committed to strong cultures of safety.

Paul "Alex" Rudd, Ph.D., feels that his work with the Joint Safety Team helped him obtain a position with BASF. "One of the first and most fundamental things that JST did was to start the tradition of the safety moment: a brief comment or reminder about some aspect of safety before all talks and seminars. These start at the group meeting level and continue through to the department seminars and even invited seminars at other universities. In the spirit of this tradition, I included a safety moment in my (20 minute) technical presentation while interviewing with BASF. The interviewers were surprised and clearly impressed that safety was an important consideration for us. In BASF, we regularly hear that, 'Safety is our license to operate,' but academia is still transitioning to this mindset. Making safety a core value and expressing this to potential employers is a win-win, and I credit it with part of my success in landing a great job," he said.

JST leaders recently made a connection with the Valspar Corporation, which, in turn, presented information on the importance of safety to first-year graduate students in both the Chemistry and CEMS departments. Members of the Valspar Corporation have assisted the JST's Education and Resource Committee in developing risk assessments that are graduate-student friendly. The JST administrative leaders have also visited the Valspar Corporation to learn about its safety protocols.

Ongoing training is important. On January 13, the Joint Safety Team is hosting a mandatory department-wide Safety Event for all laboratory safety officers in both departments. This Safety Event has two parts:

Part 1: an hour-talk with representatives from the JST, Valspar Corporation, and BASE. These safety talks are directed toward acknowledg-

ing those who have demonstrated excellent safety practices, safety expectations when working in industry, and building a better safety culture.

Part 2: 1.5 hours of activities, demonstrations and practice scenarios, involving representatives from police, fire, emergency medical technicians, Department of Environmental Health and Safety, and public relations.

While the culture of safety in the chemistry department has changed, improved, and evolved over the past three years, there is always more work to be done. The JST works hard to involve students, post-doctorates, and faculty in its efforts. This includes developing a Facebook page, engaging people in safety video or poem contests, updating safety posters, creating restroom stall wall flyers with important safety tips, procedures, and information from the

bi-annual laboratory walk throughs. The JST uses anonymous learning experience reports to engage people in learning from accidents and mistakes. The JST also honors outstanding safety volunteers and laboratories that passed its annual walk-through safety inspections.

"I really enjoy working for the Joint Safety Team," said Baudhuin. "Not only am I inspired to try and make safety a more practical learning experience for everyone, but I really believe that we can be a role model for other universities interested in starting their own student-led safety initiative."

For additional information, contact the JST at jst@umn.edu, or visit its website at <http://www.jst.umn.edu>.

in MEMORIUM

Alumnus Newman Bortnick, Ph.D.

Alumnus Newman "Newmie" Bortnick, Ph.D., of Pennsylvania, died on Monday, April 20, 2015. He was 93 years old. He received his bachelor's degree in chemistry in 1941, and his doctorate in organic chemistry in 1944 from the University of Minnesota.

In 2000, he received an Outstanding Achievement Award from the University of Minnesota for his exemplary commitment and service to the university and his profession. According to the university, "his professional contributions led to the discover, development and manufacturing of plastic, which we see and use every day such as polymeric resins used in paints, coatings and clear plastics known as Plexiglas."

From 1941 to 1943, he held the Sharp Dohme Teaching Fellowship. Following his graduation, Bortnick was employed for 67 years by Rohm

and Haas Company of Philadelphia and, for two years, the Rohm and Haas division of Dow Chemical Company, starting as a research chemist and eventually rising to the position of corporate research fellow, the highest scientific rank in the company. He remained a consultant to the company until he was 89 years old. During his long and prolific career, Bortnick authored more than 100 patents, the last obtained in 2013. He also published many research articles in various scientific journals.

From 1941 until his death, Bortnick was an extremely active member of the American Chemical Society (ACS). He held numerous positions within the ACS, including Director-at-Large from 1983-88 and chairman of the Chemical Abstracts Board. He was also a Fellow of the American Association for the Advancement of Science and the Royal



Society of Chemistry, and a lifetime member of the Chemical Heritage Foundation.

His wife of nearly 70 years, Lillian Bortnick predeceased him in 2012. Survivors include one son, Karl Bortnick, and two daughters, Lynn Bergman and Wendy Lefkowich. In addition, he is survived by six grandchildren, three great-grandchildren, and many nieces and nephews.

We are grateful to the generosity of the donors who are supporting talented and deserving chemistry students through scholarships, fellowships, and awards.

Scholarships

Astronaut Scholarship from the Astronaut Scholarship Foundation

Sammy Shaker

Peteris Auzins Memorial Scholarship

Megan Stevens and Eve Zabronsky

George B. and Mary Ann Bodem Scholarship

Spenser Marling

Stanley Bonnema Scholarship

Samuel Bryson

Robert C. Brasted Memorial Scholarship

Victoria Longley

Robert C. Brasted Memorial Fund

(outstanding undergraduate teaching assistant)

Jacob Kautzky

Thomas P. DuBruij Memorial Scholarship

Stephanie Hart

Lloyd W. Goerke Scholarship

Tony Cui, Francisco Gomez, Eric Kalkman, and David Kraus

Barry M. Goldwater Scholars (2015)

Nathan Klein and Sammy Shaker

Dr. Paul F. and Patricia Guehler Chemistry Scholarship

Stephanie Breunig and Vignish Palani

Hach Chemistry Teacher Scholarship

Anthony Kort

Sally Herz Memorial Scholarship

Baila Elkin and Alec Logeman

David A. and Merece H. Johnson Scholarship

Reid Anderson, Clay Batton, Erin Duffy, Jacob Kautzky, Nathan Klein, Edward Koleski, Abbie Mozzetti, Nikki Niewold, Francis Roushar, Joshua Schmidt, Sammy Shaker, and Elena Werst

Betty A. Lewis Scholarship

Caitlin Puro

J. Lewis Maynard Memorial Prize in Advanced Inorganic Chemistry Award

Clay Batton, Stephanie Breunig, and Sammy Shaker

Wayland E. Noland Scholarship

Sean Berg, Nathan Klein, and Luke Maki

Kenneth E. and Marion Owens Scholarship

Michael Murphy

Sigma Xi Revitalizing Science Scholarship

Jeff Ting

M. Cannon Sneed Memorial Scholarship

Alexander Benson

Jane B. Spence Scholarship

Jordan Sell and Jingyang Zheng

Fellowships

3M Science & Technology Fellowship

Mary Packard

Richard D. Amelar and Arthur S. Lodge Fellowship for Outstanding Collaborative Research in Materials

Jacob "Jake" Brutman

Newman and Lillian Bortnick Fellowship

Matthew Porter

College of Science & Engineering Fellowship

Craig Van Bruggen

Robert and Jill DeMaster Fellowship

Harrison Frisk

Department of Chemistry Fellowships

(1st-year graduate students)

Beth Dewing, Anna Huff, Siu Yi Kwang, Hussnain Sajjad, Edward Rodionov, Shuyi Xie, and Borna Zandkarimi

Department of Chemistry Fellowships

(2nd-year graduate students)

Evan Anderson, Kari Kusler, James Moore, Courtney Olson, Samuel Stoneburner, Andrew Sonnenberger, and Matthew Vollmer

Diversity of Views and Experiences Fellowship

Amani Lee and Kang Xiong-Hang

Graham N. Gleysteen Fellowship in Chemistry

Jorden Johnson, Amani Lee, and Anatolii Purchel

Dr. Carl and Dorothy Krespan Chemistry Fellowship

Kang Xiong-Hang

Lester C. and Joan M. Krogh Endowed Fellowship

Beth Dewing and Xue Zhen

Frieda Martha Kunze Fellowship

Shaohong Li

Monsanto Franz Innovative Award

Grace Gast

Wayland E. Noland Fellowship in Organic Chemistry

Constance Anderson and Amy Ott

Wayland E. Noland Fellowships in Chemistry

David Goldfeld and Shaofei Ji

Overend Awards for Graduate Research in Physical Chemistry

William Isley III and Rebecca Mackenzie

Kenneth E. & Marion S. Owens Endowed Fellowship in Chemistry

Sean Dembowski

Phillips 66 Graduate Fellowship in Chemistry

Cecilia Hall

Pillsbury Robert L. Ferm Memorial Award

(outstanding teaching assistants)

Harrison Frisk, Jacob Kautzky, Curtis Payne, and Samuel Stoneburner

Dr. Venkateswarlu Pothapragada and Family Graduate Fellowship

Kajari Bera

Jane B. Spence Chemistry Fellowship

Craig Van Bruggen

John Wertz Fellowship in Chemistry

Anna Huff

Heisig/Gleysteen Chemistry Summer Research Program Fellowships (undergraduates)

Molly Andersen, Alex Ayoub, Nathan Bjerke, Stephanie Breunig, Erin Duffy, Thomas Haversang, Levi Hogan, Alex Hurben, Kadir Hussein, Eric Kalkman, Nathan Klein, Edward Koleski, Burnell Lauer, Michael McDermott, Nam Nguyen, Nikki Niewold, Vignesh Palani, Thomas Rions-Maehren, Joshua Schmidt, and Alex Wheeler

2015-16 Doctoral Dissertation Fellowships

Joshua Borycz, Laura Clouston, Ian Gunsolus, Rebecca Mackenzie, Moshen Mahmoodi, Deborah Schneiderman, Jennifer Strehlau, Evan Weitz, and Haoyu Yu

National Science Foundation Graduate Research Fellowships

Matthew Vollmer and Danielle Francis (fellowships) and Harrison Frisk, Moriana Haj, Annabelle Lee, and Courtney Olson (honorable mentions)

Individual Awards

Baxter Young Investigators Award

Andrew R. Johnson

BASF 150th Anniversary North American Science Competition—Lightweight Solutions for a Sustainable Future

Alex Mannion, Debbie Schneiderman, Marie Vanderlaan, and Tessie Panthani

Department of Chemistry Award for Doctoral Thesis Excellence (2014)

Allison Dzubak

2015 Third-year Graduate Student Research Symposium Paul B. and Gerda Ann Gassman “Beaker and Bunsen” Chemistry Graduate Student Travel Award recipients

Debanjan Dhar, Chad Hoyer, Jinbo Hu, and Megan Weisenberger

Joint Safety Team Safety Award—Post-Doctoral Associate Jennifer Laaser and Joint Safety Team Safety Laboratory Award for Spring 2015

Professor Valerie Pierre’s laboratory

Feodor Lynen Research Fellowship from the Alexander von Humboldt Foundation

Post-Doctorate Johannes Klein

Teaching Assistant Honorable Mentions

Junwei Bao, Guilhem DeHoe, Peter Dunn, Courtney Elwell, Lee Godsey, Sarah Harris, Geoffrey Li, Waqas Rasheed, CJ Smith, Ken Tritch, and Juntian Zhang

4.0 Grade Point Averages (first-year graduate course work)

Evan Anderson, Subhasree Kal, and Shu Xu

DEPARTMENT news

Department forms Chemistry External Advisory Committee



Members of the Chemistry External Advisory Board are, front row, from left, Arthur Coury, Timothy Abraham, Kristi Fjare, William Tolman (Department of Chemistry chair), Janet Zuffa, Karl Haider, and Martin Rigney. Back row, from left, Gregory Kubala, Steven Vanderboom, Florian Schattenmann (CEAB chair), Robert DeMaster, and Scott Pearson. Not pictured are John Banovetz, Paul Guehler, Daniel LeCloux, and Yong Li.

The Department of Chemistry has formed a Chemistry External Advisory Board (CEAB) that will help it pursue strategies aimed at enhancing the vitality and effectiveness of its teaching, research, service, and outreach activities.

Members of the CEAB are leading scientists from a variety of industries, and many are

University of Minnesota and Department of Chemistry alumni. Board members include Timothy Abraham, Ph.D., Cargill Inc.; John Banovetz, Ph.D., 3M; Arthur Coury, Ph.D., biomedical consultant; Robert DeMaster, Ph.D., Suntava Corporation (retired from 3M); Kristi Fjare, Ph.D., Phillips 66; Paul Guehler, Ph.D., retired from 3M; Karl Haider,

Ph.D., Bayer MaterialScience LLC; Gregory Kubala, Ph.D., Schlumberger Pressure Pumping and Chemistry; Daniel LeCloux, Ph.D., DuPont Microcircuit Materials; Yong Li, Ph.D., Eastman Chemical Company; Scott Person, Ph.D., Coca-Cola Company; Martin Rigney, Ph.D., Ecolab; Florian Schattenmann, Ph.D., Dow Chemical Company; Steve Vanderboom, Pace Analytical Services Inc.; Janet Zuffa, Ph.D., Masonite Corporation. Schattenmann serves as the CEAB chair.

The CEAB will advise the department on academic, program, and strategic issues; assist in the promotion and recognition of the department; and provide philanthropic support and assistance in seeking public and private financial support. The CEAB will meet twice a year.

“We are very pleased with the commitment to our efforts from these very busy and successful people, and I look forward to working with them over the coming years,” said Professor William Tolman, department chair.

Sammy Shaker receives prestigious Astronaut Scholarship



Sammy Shaker

Sammy Shaker, one of the Department of Chemistry's top undergraduate students and a College of Science & Engineering and University Honors Program student, received a prestigious \$10,000 scholarship from the Astronaut Scholarship Foundation. The

Astronaut Scholarship is the largest merit-based scholarship program in the nation for undergraduate students in science, technology, engineering and mathematics fields.

Sammy is majoring in chemistry and mathematics and hopes to pursue a doctorate in inorganic materials chemistry. He plans to work in several areas of novel material synthesis and characterization to address problems in energy storage and conversion as well as heterogeneous catalysis.

He has been taking classes and conducting research since coming to the university four years ago through the state's Post-Secondary Education Options. While still in high school, Sammy began doing research at the university with Mathematics Professor Duane Nykamp, modeling neural networks. Since his freshman year, he has worked in the laboratory of Chemistry Professor Andreas

Stein to develop templates for synthesizing porous and nanostructured materials. He has worked with Mathematics Professor David Clark to solve a problem of error-correcting codes, and with Professor Robert Tranquillo to analyze particle image velocimetry for a tissue-engineered heart valve. He also worked on a project for abdominal ultrasounds in the context of cholecystitis with Dr. Brian Driver at the Hennepin County Medical Center (HCMC).

One of his projects in Professor Stein's laboratory involved the morphology control of porous, redox active metal oxides for solar thermochemical water splitting. This work has resulted in a publication in the journal *Inorganic Chemistry*, with Sammy as one of the co-authors.

"Sammy is an extraordinarily gifted student," said Stein, "of the type whom I have met only once or twice in my career. He has taken a degree of ownership for his undergraduate research projects that you expect only from advanced graduate student. His command of technical language as well as his insightful questions and suggestions, simply amaze me. Sammy is an exceptional student with a prospect for a brilliant career."

Sammy has earned a number of awards, scholarships and fellowships while at the university, including the prestigious honor of being named a Goldwater Scholar. Some of his other honors



Sammy Shaker received his Astronaut Scholarship award from Minneapolis native Robert Cabana, a Hall of Fame astronaut and current NASA Kennedy Space Center Director.

include a National Merit Scholar-Walgreens Corporation, Bentson Family Scholar, Winchell Excellence in Science Award, Gold Scholarship, Presidential Scholarship, CRC Freshman Chemistry Award, CHEM 1021 General Chemistry Award, Jane B. Spence Scholarship, M. Cannon Sneed Scholarship, J. Lewis Maynard Memorial Prize in Advanced Inorganic Chemistry Award, David A. and Merece H. Johnson Scholarship, American Chemical Society DIC Travel Award, and Heisig/Gleysteen Chemistry Summer Research Program Fellowships. A native of Roseville, MN, he is active in the Shotokan Karate Club and the Al-Madinah Cultural Center.

Professor Emeritus Doyle Britton

Professor Emeritus John Doyle Britton "Doyle" died in Minneapolis on Tuesday, July 7, at the age of 85. He was born on March 6, 1930 in Los Angeles, CA.

Britton earned his bachelor's degree in chemistry and mathematics from the University of California, Los Angeles, in 1951, and his doctorate from the California Institute of Technology in 1955. He joined the University of Minnesota Department of Chemistry in 1955 and retired 44 years later in 1999.

He focused on inorganic chemistry and specialized in crystallography.

Britton had a reputation as being a kind, gentle and caring man, and was a treasured professor in the department. He was also somewhat of a Renaissance man—an athlete (lettering in water polo as an undergraduate), scientist, lover of poetry and literature, mountain climber, and traveler.



He is survived by his loving wife of 52 years, Judy G.; children, Jenny, David (Amy) and Mary Katherine; grandchildren, Seth, Joe

and Eli; nephews, Don (Jennifer) Hirsh, Tom (Deb) Hirsh; nieces, Paula (Dave) Koeller, Bonnie Reibman; relatives, co-workers and friends.

Two Goldwater Scholars



Nathan Klein

The Department of Chemistry has not one, but two, Goldwater Scholars. In addition to Sammy Shaker, **Nathan Klein** of Lakeville, MN, also received a 2015 Goldwater Scholar. He is majoring in chemistry and mathematics, and plans to complete a doctorate in analytical chemistry.

As a professor at a research university, he intends to develop analytical techniques that will help to solve problems in public health, particularly issues related to allergic responses. Educated at home, he began taking courses in math and chemistry at the University of Minnesota at age 14. With his sister, he developed a summer science program for kids. In the future, he hopes to inspire college students to be excited about science and to become scientifically literate citizens.

Klein works in the lab of Professor Christy Haynes on heat-mediated drug release from inorganic nanoparticles, where he is developing a new method to analyze cellular internalization of inorganic nanoparticles using electron microscopy. He has also conducted research on heterocyclic Diels-Alder reactions in the lab of Professor Wayland Noland.

Nathan has great scientific instincts and is creative, said Professor Haynes. "One recent illustration of Nathan's creativity is that he had a great idea about using dark field imaging with transmission electron microscopy (TEM) to analyze some complex samples in my lab. He first brought up this unusual imaging modality right after he was trained on this instrument. His instincts were right. It turns out that we can use dark field mode on the TEM to look for strongly-diffracting nanoparticles in what would otherwise be extremely noisy environments such as tissue, cells, and natural organic matter. Since his initial suggestion, he and his graduate student

mentor, Katie Hurley [who has now earned her doctorate], have implemented this technique to analyze bacteria samples, tumor slices, and silver nanoparticles in natural organic matter, making contributions to both his own project and those of others in my research group. A manuscript in which Nathan is a co-first author was accepted for publication in *Analytical Chemistry*. Very few people use dark field in general, and no one has used it on biological samples before—this opens up a lot of new, exciting possibilities based on Nathan's scientific instincts," she said.

Klein is a National Merit Scholar, a member of Phi Beta Kappa, and a member of the University of Minnesota unicycle club. His awards include a David A. and Merece H. Johnson Scholarship, Robert C. Brasted Memorial Scholarship, the Gayle W. McElrath Memorial Scholarship, ADC Scholarship, and an Undergraduate Research Scholarship.

Klein receives Feodor Lynen Research Fellowship

Post-doctoral Associate Johannes Klein received a prestigious Feodor Lynen Research Fellowship from the Alexander von Humboldt Foundation. Klein is working in the laboratory of Regents Professor Lawrence Que Jr.

With a strong interest in interdisciplinary research, Klein is combining his core training in organic chemistry with opportunities to focus on bioinorganic chemistry in Que's laboratory. His current research focuses on the preparation and study of high-valent iron complexes, and how these can be applied to the selective oxidation of organic matter resulting in valorization.

Klein received his Bachelor of Science degree from the Universität Dortmund in Germany,

and his master's degree from University College in Dublin, Ireland. In 2014, he earned his doctorate from the Universität Stuttgart in Germany, under the tutelage of Professor Bernd Plietker.

The purpose of the Feodor Lynen Research Fellowship is to promote academic cooperation between excellent scientists and scholars from abroad and from Germany. Fellowship recipients must be supported, or what's called hosted, by Humboldt Foundation alumni, who are called Humboldtians. Klein's host is Department Chair William Tolman who received a Humboldt Foundation Research Award in 2004.



Johannes Klein

Two important research centers receive ongoing funding

Collaborative multidisciplinary research continues for Materials Research Science and Engineering Center, and the Center for Sustainable Nanotechnology

Department of Chemistry researchers work with a number of multi-disciplinary, collaborate research centers that are fund by the Department of Energy, National Science Foundation (NSF), and National Institutes of Health. Two important centers received new funding grants in 2015.

The NSF renewed, for the third time, grant funding for the 16-year-old Materials Research Science and Engineering Center (MRSEC). The new six-year grant is \$17.8 million. It was originally funded in 1998, with grants renewed in 2002 and 2008. The university's MRSEC is directed by Timothy Lodge, a Regents Professor in both the Department of Chemistry and the Department of Chemical Engineering and Materials Science.

NSF MRSECs support interdisciplinary and multidisciplinary materials research that addresses complex problems in science and engineering, which are important to society, and

which could not be addressed under traditional funding of individual research projects. The university's MRSEC has three distinct foci, clustered in what are called Interdisciplinary Research Groups (IRG). These IRGs involve 27 faculty researchers from five different departments in the highly-collaborative College of Science & Engineering, including Chemistry, Chemical Engineering and Materials Science (CEMS), Electrical and Computer Engineering, Mechanical Engineering, and Physics.

Professor Chris Leighton from CEMS is coordinating the research group, Electrostatic Control of Materials. Professor Uwe Kortshagen from the Department of Mechanical Engineering is coordinating the research team, Sustainable Nanocrystal Materials. Chemistry Professor Christy Haynes is one of the researchers exploring the environmental stability and toxicity of new nanocrystal materials in this IRG.

Chemistry Professor Theresa Reineke is leading the third IRG, Hierarchical Multifunctional Macromolecular Materials, concentrating on assembling polymeric materials with superior properties that can be used for a variety of diverse applications such as water treatment, fuel cell membranes, gene therapy, and intricate circuit manufacturing. Department of Chemistry professors Lodge, Marc Hillmyer, and Ilja Siepmann are also involved in a number of specific research efforts in this IRG.

The University's MRSEC also helps researchers with its seed program, providing grants of \$50,000 for innovative research. Chemistry Professor James Johns received a seed grant to research the ultrafast photoemission of suspended 2D materials.

Center for Sustainable Nanotechnology

University of Minnesota researchers are part of a team of researchers from the Center for Sustainable Nanotechnology (CSN) who received a new \$20 million grant from the National Science Foundation to evaluate the impact of nanotechnology on the environment and living things. Professor Christy Haynes, a leading researcher in the growing field of nanotoxicology, is the center's associate director. The multi-institutional research center is based at the University of Wisconsin-Madison.

Nanotechnology involves the use of materials at the smallest scale, including the

manipulation of individual atoms and molecules. Products that use nano-scale materials range from beer bottles to car wax, solar cells, and electric and hybrid car batteries. While there are already hundreds of products that use nanomaterials in various ways, much remains to be learned about how nanoparticles affect the environment and the multitude of organisms—from bacteria to plants, animals and people—that may be exposed to them.

One of the new principal investigators joining the CSN team is Chemistry Professor Erin Carlson. With expertise in molecular

synthesis and mass spectrometry, Carlson brings tools and techniques that will help the team to investigate and control molecular-level chemical and biological interactions with nanoparticles.

The general public can engage with the CSN's research progress and activities through the CSN's blog at <http://sustainable-nano.com/>.

New Faculty

Expertise in synthesis of natural products, and application of new electronic structure techniques.

Professor Joseph Topczewski

Joseph Topczewski, Ph.D., joined the Department of Chemistry as an assistant professor, starting in July 2015. Previously, he was a National Institutes of Health post-doctoral fellow at the University of Michigan, working with Professor Melanie Sanford. He also was a post-doctoral scholar at the University of Iowa, working with Professors Hien Nguyen and Daniel Quinn. Topczewski earned his doctorate in organic chemistry from the University of Iowa under the tutelage of Professor David Wiemer. He received his bachelor's in chemistry from the University of Wisconsin at Parkside.

As a graduate student, Topczewski completed the total synthesis of several anti-proliferative natural products after developing a cascade cyclization to enable the synthesis. Subsequent

medicinal chemistry efforts elaborated a structure activity profile. As a post-doctoral scholar, Topczewski focused on developing efficient catalytic methods to enable key bond formations central to biologically active molecules. These efforts included C-F (aryl and alkyl) bond formations with the PET radioisotope ^{18}F and the distal C-H activation of piperidines.

At the University of Minnesota, Topczewski is interested in designing and understanding inherently green reactions to enable sustainable synthesis. His research focuses on developing direct catalytic methods of molecules of proven value, developing renewable approaches to feedstock chemicals, and in quantifying improvements in these processes with sustainability metrics.



Professor Joseph Topczewski

Jason Goodpaster, Ph.D.

Jason Goodpaster, Ph.D., is joining the Department of Chemistry as an assistant professor, starting in the summer of 2016. Since September 2014, he has been a post-doctoral researcher at the Joint Center for Artificial Photosynthesis at the Lawrence Berkeley National Laboratory, working with Professors Martin Head-Gordon and Alexis Bell. Goodpaster earned his doctorate in chemical engineering from the California Institute of Technology under the tutelage of Professor Thomas F. Miller III. He received his bachelor's degree in chemical engineering from the University of Illinois Urbana-Champaign.

Goodpaster's current research focus is on the fundamental quantum chemical modeling of CO_2 reduction. This project aims to contribute mechanistic insight from electronic structure computations on experimentally relevant systems, as well as attempting to give insights that can impact the design principles for future

catalysts. In support of this main objective, the project includes the development of new computational methods used for the modeling of electrochemical reactions.

As a graduate student, Goodpaster's research project centered on the development and application of quantum embedding theories. This approach allows for accurate calculations to be performed on large complex systems while remaining computationally efficient.

At the University of Minnesota, Goodpaster is interested in the development, implementation, and application of new electronic structure techniques. His research will focus on the development of multi-scale methods, which allow for the study of large and extended systems. He is specifically interested in applying these new methods to metalloenzymes, heterogeneous catalysts, and metal-organic frameworks.



Jason Goodpaster, Ph.D.

Solving issues that have an impact on society drives the work of researchers

Whether it is the advent of the space race, or an early and persistent interest in science, chemistry has long engaged the passion of two prominent scientists, Theresa Reineke and Donald Truhlar.

Theresa Reineke



Professor Theresa Reineke

Professor Theresa Reineke can't remember a time when she didn't love science. Even as a little girl, she wanted to be a scientist or engineer.

A first-generation college student, Reineke credits her parents and

high school teachers/coaches for their inspiration, fostering her interest in chemistry, and instilling in her a strong work ethic. A science-focused demonstration show at the University of Minnesota also made her think, "Really, I can do this." A multi-sport athlete at Park High School in Cottage Grove, Reineke's involvement in competitive athletics also helped her learn what it means to be part of collaborative teams.

At the University of Wisconsin-Eau Claire, because of her deep love for all science, Reineke found it hard to determine what fields to pursue. She sampled a variety of science courses

from different foci such as geology, astronomy, chemistry and physics, before settling on a chemistry major and physics minor.

After receiving her bachelor's degree, Reineke earned her master's degree in chemistry from Arizona State University, and her doctorate in chemistry from the University of Michigan. Her graduate degree adviser was Omar M. Yaghi. Under his tutelage, Reineke studied the synthesis and characterization of metal-organic framework materials. After completing her doctorate, she received a National Institutes of Health (NIH) National Research Service Award to study the synthesis and biological characterization of carbohydrate-containing polymers for gene therapy. She conducted this research as a post-doctoral fellow in Mark Davis' laboratory at the California Institute of Technology. One of the polymers that she helped to optimize in the Davis lab went on to be the carrier for the first siRNA drug to complete Phase I human clinical trials.

Before coming to the University of Minnesota in 2011, she was an associate professor of chemistry at Virginia Tech, and an assistant professor of chemistry and Lowenstein Scholar



Theresa Reineke and her husband Dr. Jeff Reineke have two children, Abigail, 6, and Jacob, 10.

at the University of Cincinnati. She also was an analytical chemist at Upsher-Smith Pharmaceuticals in Minneapolis for a year. Currently, Reineke is the Department of Chemistry's Lloyd H. Reyerson Professor of Chemistry.

She has expertise in polymer science, drug delivery, gene therapy and diagnostics. Reineke is a world leader in the area of polymer/deoxy-ribonucleic acid nanostructures for medical applications. Her research group members specialize in the synthetic design, chemical characterization, and biological study of sophisticated macromolecules. They seek to discover novel polymeric vehicles and strategies to safely deliver nucleic acids and drugs, impart enhanced material performance from sustainable feedstocks, and elucidate cellular-level mechanisms in biomaterials and animals.

In her four years at the University of Minnesota, Reineke's research interests have broadened and morphed due to the diverse, multi-disciplinary collaboratives that she is

"You have to have one foot in the fundamentals of your discipline, and one foot willing to step into different areas of expertise that are needed to address some of the important challenges our society is facing."

—Professor Theresa Reineke

involved with including the Materials Research Science and Engineering Center (MRSEC), the Center for Sustainable Polymers, and the Center for Genome Engineering.

Reineke is leading one of MRSEC's interdisciplinary research groups, Hierarchical Multifunctional Macromolecular Materials, concentrating on assembling polymeric materi-

als with superior properties that can be used for a variety of diverse applications such as water treatment, fuel cell membranes, gene therapy, and intricate circuit manufacturing.

From chemistry to chemical engineering, from materials science to cell biology, Reineke believes strongly that research needs to be interdisciplinary and collaborative. Students in

her lab are routinely exposed to diverse training and research in several areas such as chemistry, chemical biology, materials science, and engineering.

"You have to have one foot in the fundamentals of your discipline, and one foot willing to step into different areas of expertise that are needed to address some of the important challenges our society is facing," she said.

Reineke has an entrepreneurial spirit, which has lead her to work with industries such as Dow Chemical Company. She is principal investigator and director of the Dow Actives Research Partnership aimed at developing new polymer-based drug-delivery vehicles. This partnership is dedicated to unraveling the intricate design parameters needed to advance oral delivery of poorly soluble/bioavailable therapeutics such as anti-cancer and anti-seizure medicines.

Reineke enjoys working on major challenges, particularly, health care issues. For example, it is possible that genome editing may lead to customization of medicines to attack specific acquired and inherited diseases such as cancer and muscular dystrophy.

"It is exciting and inspiring to work on issues like these," she said.

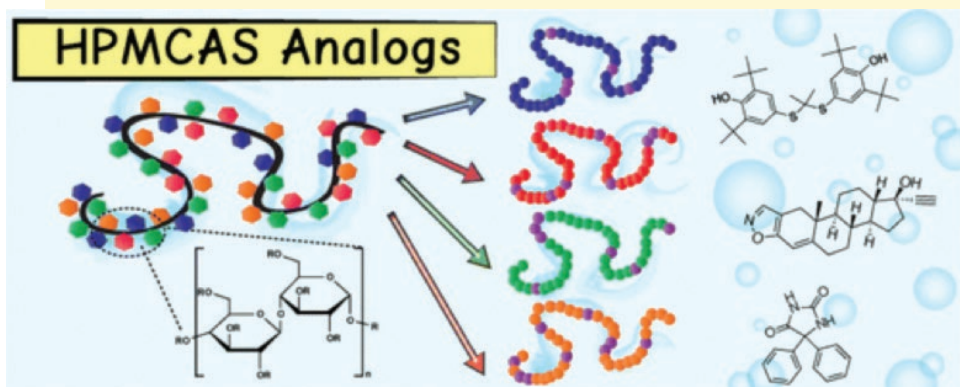
For Reineke, one of the favorite parts of being a professor is mentoring young people, ranging from showing young people how fun and important science is and encouraging them to go to college, to shepherding students through five years of graduate school and then helping them launch scientific careers and become experts in their field as faculty members, teachers, and researchers in industry.

"It makes me proud to teach students and to see them become successful scientists on their own," Reineke said. "It is privilege to work with the interesting people, of all ages and backgrounds, that I have worked beside throughout my career," she said.

She believes in contributing to the profession. Reineke serves as a founding associate editor for *ACS Macro Letters*, and is on the editorial

Theresa Reineke Research

Researchers benchmark tunable polymers for oral drug administration



Professor Theresa Reineke is an outstanding researcher with expertise in polymer science, drug delivery, gene therapy, and diagnostics.

Oral drug delivery is the most widespread and desirable form of administration for patients worldwide. Unfortunately, many new drug molecules suffer from poor water solubility, an enormous challenge to efficiency and reliability in overall therapeutic delivery to molecular targets. In response, researchers at the University of Minnesota have partnered with the Dow Chemical Company to formulate new polymeric materials to better understand and overcome this key issue. Researchers from the Professor Theresa Reineke and Professor Frank Bates labs have developed a well-defined synthetic polymer platform and examined its utility with several model drugs at various dosages, which exhibited promising delivery performances with high levels of drug solubilization. Moreover, key structure-property relationships have been systematically identified to enable future development of rationally-designed delivery systems. Their publication, "Deconstructing HPMCAS: Excipient Design to Tailor Polymer-Drug Interactions for Oral Drug Delivery," has been published in *ACS Biomaterials Science & Engineering* and was selected as an American Chemical Society Editors' Choice Article, allowing open access of their work to the global community of researchers. The Dow Chemical Company has also worked with the University of Minnesota to file and license this technology through two related world patent applications entitled, "Sugar containing, amphiphilic copolymers," and "Sugar free, statistical copolymer made from at least three monomers."

advisory boards of *Bioconjugate Chemistry*, *Biomacromolecules*, and *Macromolecular Bioscience*. She serves as publicity chair for the American Chemical Society (ACS) Division of Polymer Chemistry, and is the founding faculty adviser for the ACS POLY/PMSE Division University of Minnesota Student Chapter. She has also served as chair of the Molecular Conjugates Committee of the American Society of Gene and Cell Therapy.

Reineke has received numerous awards for her research, including a Beckman Young Investigator Award, a Sigma Xi Outstanding

Young Investigator Award, a Camille Dreyfus Teacher-Scholar Award, a National Science Foundation Career Award, an ACS Arthur K. Doolittle Award, a National Institutes of Health Director's New Innovator Award. She is also a recipient of the Alfred P. Sloan and Kavli Fellowships. In addition, Reineke has six patents, and another six patents pending stemming for her work at the University of Minnesota. She has written more than 100 scientific articles and delivered more than 130 invited lectures on her research.

Outside of her work at the university, Reineke's greatest joy is her family, and her favorite way to relax is spending time with family and friends. In 2016, she will celebrate her 20th wedding anniversary with husband Jeff Reineke, Doctor of Osteopathic Medicine (D.O.), who is a technology liaison/research and development engineer at Boston Scientific. They have two children, Jacob, 10, and Abigail, 6. She also still enjoys being an athlete, running, lifting weights, hiking, and biking. She was recently inducted into the Park Senior High Athletic Hall of Fame for track and field.



Regents Professor
Donald G. Truhlar

Donald Truhlar

In 1957, when the Russians launched Sputnik I, the first artificial Earth satellite, it sparked a strong interest in physics in this country. Regents Professor Donald G. Truhlar, after graduating from high school in his

native Chicago, followed his brother John to St. Mary's College in Minnesota where both of the Truhlar brothers initially majored in physics.

"But I switched to chemistry because of the very interesting carbene research being conducted by Brother Philip Hogan, who was an inspirational teacher of organic chemistry," said Truhlar. "At one point, after completing organic chemistry and finding that analytical

chemistry was not my cup of tea, I considered switching back to physics, but I was talked out of that by my second undergraduate research adviser Professor Ernest D. Kaufman."

He earned his bachelor's degree in chemistry from Saint Mary's College (now St. Mary's University of Minnesota) in 1965. With a fellowship offer for graduate school from the California Institute of Technology (Caltech), Truhlar married Jane Gust in her hometown of Crookston, MN, and that same day, they headed west in his almost-new Chevrolet.

As a graduate student at Caltech, Truhlar joined the experimental group of Professor Aron Kupperman to do photochemistry experiments. However, he quickly became more interested in using quantum mechanics to explain the dynamics than in doing the measurements. By the end of his first year in graduate school, Truhlar was a theoretical chemist with a plan to develop methods for calculating the

dynamics of chemical reactions. He earned his doctorate in 1970. Truhlar also (much later) received a Doctor honoris causa from Technical University of Lodz, Poland.

Truhlar joined the Department of Chemistry faculty in 1969. He wanted to return to Minnesota because it was the home of Control Data Corporation, which was making powerful scientific computers that eventually evolved into the first supercomputers designed by Seymour Cray—the father of supercomputing. The University of Minnesota had a CDC computer.

Thanks to computational theorists like Truhlar, Minnesota has long been a leader in high performance supercomputing. It was the first university in the United States to obtain a supercomputer in 1981, and in 1984, it formed the Minnesota Supercomputer Institute (MSI) for advanced computational research. Truhlar is a MSI Fellow and, for 18 years, he served as director of the MSI.

"Minnesota also had a robust and active theoretical chemistry group with Alden Mead, Al Moscovitz, Steve Prager, John Dahler, Ted Davis, and Fred Van-Catledge," said Truhlar. "It was very exciting to join that thriving and enthusiastic group of theorists."

Truhlar worked with graduate students and post-doctoral associates to develop new methods for calculating the converged quantum

"I think we have the best theoretical chemistry group in the world, and it is very exciting to be a part of it."

—Regents Professor Donald Truhlar

dynamics of chemical reactions and to use them to calculate accurate quantum mechanical reaction cross sections and rate constants from first principles. This work combined new theory, new algorithms, and state-of-the-art computing to calculate chemical dynamical reaction rates and reaction cross sections that allowed theory to compete with experimental chemistry.

Truhlar and his students and collaborators also worked on several other projects. "I was fortunate to engage in several long-term collaborations, including variational transition state theory with Bruce Garrett, solvation modeling and charge modeling with Christopher Cramer, and enzyme kinetics with Jiali Gao," said Truhlar. "I am very proud to be associated with the current theoretical chemistry group (Cramer, Laura Gagliardi, Gao, Jason Goodpaster, and Ilja Siepmann) in the Department of Chemistry. I think we have the best theoretical chemistry group in the world, and it is very exciting to be a part of it."

Today, Truhlar is one of the University of Minnesota and Department of Chemistry's most distinguished professors and researchers with a long record of service to the university, the Department of Chemistry, and to his profession. In 2006, he was named a Regents Professor, the university's highest faculty honor. In 1998, he received the George W. Taylor Award for Distinguished Service, recognized for his outstanding service to the university and service to governmental or other groups.

Truhlar's teaching and advising record is unparalleled. He has taught numerous graduate and undergraduate courses, and he has mentored 144 graduate students and post-doctoral associates and 70 undergraduate research students. He has been honored for his roles as a mentor and adviser with the Graduate and Professional Student Assembly Outstanding Adviser Award and the Council of Graduate Students Outstanding Faculty Award.

"It is my privilege to work with many talented graduate students and post-doctoral associates," said Truhlar. "We work closely together on our projects, and we have many group meetings and subgroup meetings as well as

Donald Truhlar Research

New high level for photochemical dynamics of complex systems

"Photodissociation Dynamics of Phenol: Multi-State Trajectory Simulations including Tunneling," X. Xu, J. Zheng, K. R. Yang, and D. G. Truhlar, *Journal of the American Chemical Society* 136, 16378-16386 (2014). [dx.doi.org/10.1021/ja509016a](https://doi.org/10.1021/ja509016a)

This paper establishes a new high level for photochemical dynamics of complex systems. It does this by combining four state-of-the-art methods in a complementary way:

- the fourfold way for diabatic states, originally published in the *Journey of Chemical Physics* in 2001-02. This is the only generally successful method for generating global diabatic potential energy surfaces; the application to phenol was published in the *Journal of Chemical Theory and Computation* in 2013.
- anchor points reactive potentials, originally published in *Journal of Chemical Theory and Computation* in 2014. The application to fitting potentials for a complex system was originally published in *Chemical Science*, where the application target was phenol; this yields useful, high-level full-dimensional potential surfaces and couplings for a reactive system with 33 internal degrees of freedom, going beyond precedents by a large margin.
- coherent switches with decay of mixing, originally published in the *Faraday Discussions* and *Journal of Chemical Physics* in 2004. This method includes density matrix coherence and decoherence and appropriate, but hard-to-obtain, insensitivity to representation, both sorely missing in competitive methods.
- army ants tunneling, originally published in *Chemical Science* in 2014, with an extension to electronically nonadiabatic simulations published in *Journal of Physical Chemistry Letters* in 2014. This method, after years of unsuccessful attempts by leading dynamicists, finally establishes a way to include tunneling in molecular dynamics simulations by taking advantage of what Truhlar and his group have learned by including multidimensional tunneling in variational transition-state theory.

Truhlar said: "This paper represents the culmination of an effort extending over more than a decade, finally coming to fruition in a dramatic way, and that is the first thing that makes it particularly satisfying to me. In the paper cited, we combined these four advances for the first time, and we applied the combined method to a prototype problem in photochemical dynamics, namely the widely studied photodissociation of phenol, which involves two separate conical intersections and proceeds entirely by tunneling. Our dynamics calculations agree well with the experimentalists' hard-won kinetic energy distributions, but they also reveal a host of details, some very surprising, about what is happening at the atomic level, demonstrating the power of theory to unravel complex photochemical dynamics and also providing long-sought information about what precisely is happening in the system. The second thing I like about this paper is that I believe it opens new doors for future detailed study of photochemistry by quantum mechanics, and that is a subject we are currently pursuing in my research group."



Regents Professor Donald G. Truhlar was inducted into the American Academy of Arts and Sciences, Saturday, October 10, 2015.

one-on-one meetings, where we can discuss details of the work. They are very motivated and creative, and I learn a lot from them,” he said.

Truhlar is one of the top physical chemists in the world. He has received many prestigious awards and honors for his research and his seminal contributions that have advanced and transformed chemistry and chemical physics, which includes publishing more than 1,100 papers and book chapters. According to Google Scholar Citations, his publications received their 100,000th citation on September 27, 2015. Truhlar has an h index of 140, denoting 140 publications with 140 or more citations. This is believed to be the second highest h-index of any theoretical chemist in the entire history of the field, trailing only the h-index of Nobel Laureate Martin Karplus.

For Truhlar, it is hard to pinpoint one particular research highlight. Perhaps the most exciting single research finding Truhlar ever had was discovering that the quantized transition state vibrational energy level structure was actually physically observable.¹ Quantized transition state features were identified in the accurate quantum dynamics for several reactions based on calculations of the microcanonical rate constants. The new approach revealing these states most clearly is the calculation of the density of reactive states.

“We found that, individually, the quantized levels of the transition state gate the reactive flux with near unit efficiency, and that, together, they globally control chemical reactivity for the entire range of energies relevant to

thermal rate constants up to high temperature,” Truhlar said. “We eventually showed that the transition state energy levels are resonances, in the language of scattering theory, or poles of the scattering matrix, in more mathematical language. This interpretation of exact quantum mechanical results provides a foundation for approximate theories such as variational transition-state theory, which are based on the postulate that quantized

transition states control chemical reactivity. In addition, the propensities for selected reactant states to react via particular levels of the transition state provided a more detailed understanding of state-selected reactivity trends.”

The future of computational chemistry holds amazing promise, Truhlar said. “Computational science holds tremendous promise for simulating complex systems in a way that will become more and more powerful, replacing experimental work as the primary way to learn about nature in more and more subfields.”

Respected and honored national and internationally, some of Professor Truhlar’s numerous honors and awards include the prestigious American Physical Society 2016 Earle K. Plyler Prize for Molecular Spectroscopy and Dynamics, American Chemical Society (ACS) Award for Computers in Chemical and Pharmaceutical Research, American Chemical Society Peter Debye Award for Physical Chemistry, Schrödinger Medal of The World Association of Theoretical and Computational Chemists, Dudley R. Herschbach Award for Excellence in Research in Collision Dynamics, Royal Society of Chemistry Chemical Dynamics Award, National Academy of Sciences Award for Scientific Reviewing, Distinguished Alumnus Award of St. Mary’s University of Minnesota, and the Minnesota Award of the Minnesota Section of the ACS. In 2006, the *Journal of Physical Chemistry* published a Festschrift in his honor and, in the spring of 2015, the American Chemical Society honored his research contributions

with a symposium for his contributions to and advancement of theory and computation in the understanding of the structure, energetics, and dynamics of molecules in gas phase, macromolecular, and condensed-phase systems.

His contributions to the scientific community include serving as an associate editor for the *Journal of the American Chemical Society* and editor of *Computer Physics Communications*. He is also past editor of *Theoretical Chemistry Accounts* and currently serves as chief advisory editor of that journal as well as on several other editorial boards. He was recently honored by the American Physical Society as an Outstanding Referee of the *Physical Review* and *Physical Review Letters*, recognized for his help in assessing manuscripts for publication, and for providing invaluable reports and advice to authors, researchers, students, and readers.

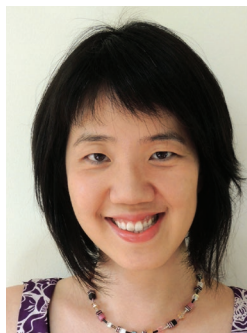
Truhlar is a member of the National Academy of Sciences of the United States of America, and the International Academy of Quantum Molecular Sciences. He is a Fellow of the American Academy of Arts and Sciences, the American Association for the Advancement of Science, the American Physical Society, the American Chemical Society, the Royal Society of Chemistry, and World Association of Theoretical and Computational Chemists, and is an Honorary Fellow of the Chinese Chemical Society.

Truhlar loves his family immensely. He married his wife Jane in 1965, “who is not only talented, but also beautiful,” he said. “My wonderful daughters Sara and Stephanie are also very successful, and I have two outstanding sons-in-law. Each of my daughters’ families includes a son. My grandson Sam was born in October 2010, and my grandson Luke was born in October 2015.” His older brother John is a retired physicist/financial adviser, and his younger brother Bob is a nationally honored employment-law attorney.

¹“Global Control of Suprathreshold Reactivity by Quantized Transition States,” D. C. Chatfield, R. S. Friedman, D. G. Truhlar, B. C. Garrett, and D. W. Schwenke, *Journal of the American Chemical Society* 113, 486-494 (1991).

Faculty Promotions

Two Department of Chemistry professors were promoted in 2015—Lee Penn from associate professor to professor, and Connie Lu from assistant professor to associate professor with tenure.



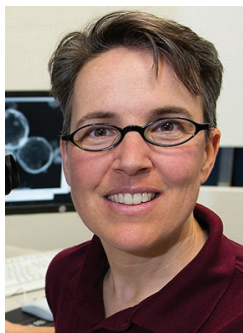
Connie Lu

Connie Lu

Connie Lu joined the Department of Chemistry faculty as an assistant professor in 2009. She earned her bachelor's degree in chemistry from the Massachusetts Institute of

Technology in 2000, and her doctorate in chemistry from the California Institute of Technology in 2006. She was the Alexander von Humboldt Post-Doctoral Fellow, working at the Max Planck Institute for Bioinorganic Chemistry for three years before coming to the University of Minnesota.

Researchers in her laboratory seek to develop homogeneous catalysts for converting abundant small molecules, such as N_2 and CO_2 , into useful chemical feedstocks such as ammonia and methanol. Current projects focus on developing highly tailored bimetallic active sites for both homogeneous and heterogeneous catalysis.



Lee Penn

Lee Penn

Lee Penn joined the Department of Chemistry faculty as an assistant professor in 2001 and was promoted to associate professor with tenure in 2008. She earned a bachelor's degree in

chemistry from Beloit College in 1992, and her master's degree in 1994 and doctorate in 1998 from the University of Wisconsin-Madison. She was an adjunct faculty member at Towson University for a year, and then was a post-doctoral researcher at Johns Hopkins University for a year before coming to the University of Minnesota.

Her research focuses on four major areas, including:

- elucidating the fundamental aggregation and growth mechanisms, especially nonclassical crystal growth mechanisms, of inorganic nanoparticles;
- characterizing the chemical reactivity of natural and synthetic nanoparticles;
- characterizing the magnetic behavior of iron oxide nanoparticles (e.g., natural and synthetic ferrihydrite, goethite, and magnetite); and
- designing and implementing effective curriculum introducing atomic-structure imaging in a high-resolution transmission electron microscope as a means to strengthen and improve middle school students' understanding of the atomic structure of solid materials.

CSP team wins BASF Science Competition

A team of graduate student researchers—Alex Mannion, Tessie Panthani, Debbie Schneiderman, and Marie Vanderlaan—won the BASF 150th Anniversary North American Science Competition: Lightweight Solutions for a Sustainable Future. They work with the Center for Sustainable Polymers (CSP) and are from the departments of Chemistry and Chemical Engineering & Materials Science (CEMS).

BASF's challenge focused on the question of what chemistries can be used to create lightweight solutions with improved end of life management. The competition was designed to encourage innovative and game-changing ideas that address lightweight challenges in three areas—food, smart energy, and urban living. The CSP researchers' project was on sustainable polyurethane foams. They were one of five teams that won \$5,000 to support their project and chosen to present their concept to BASF executives.

As the winning team, they received an all-expense paid trip to BASF International Summer Course in Ludwigshafen Germany, which was an opportunity to meet with other young scientists from around the world, to gain insight into an international company, and to learn about the broad field of research and technology activities, strategies, innovation management and other topics.

Schneiderman and Vanderlaan are advised by Professor Marc Hillmyer, Alex Mannion is advised by Professors Frank Bates and Chris Macosko, and Tessie Panthani is advised by Professor Bates.

FACULTY & STAFF honors & awards

George Barany

Professor George Barany was awarded the *2015 Murray Goodman Scientific Excellence & Mentorship Award* from the American Peptide Society. He was honored “for his pioneering and seminal contributions to new synthetic methods for peptide and protein synthesis, and for his exceptional and generous mentorship of outstanding peptide scientists.” Barany is internationally recognized for his pioneering development of mild methods for solid-phase synthesis of peptides, the co-invention of DNA-on-a-chip technology, and the introduction of the concept of orthogonality into organic chemistry and chemical biology.

Philippe Buhlmann

Professor Philippe Buhlmann received a *2015 award for Outstanding Contributions to Graduate and Professional Education*. He has been a professor and researcher in the Department of Chemistry for 15 years, teaching and developing courses, and mentoring 75 undergraduates in research. Buhlmann has served as the Director of Graduate Studies since 2012. He leads the Chemists in the Library outreach program for the Minnesota Local Chapter of the American Chemical Society (ACS), and engages high school students in research through the ACS SEED summer program. He coordinated the department’s summer undergraduate research program for seven years, and is principal investigator of a National Science Foundation grant to support summer undergraduate research.

Department of Chemistry

The Department of Chemistry is ranked **29th in the world in chemistry** in the 2015 the Academic Ranking of World Universities (ARWU), which was released by the Center for World-Class Universities (CWCU) of Shanghai Jiao Tong University. ARWU uses six indicators to rank world universities, including the number of alumni and staff winning Nobel Prizes and Fields Medals, number of highly-cited researchers selected by Thomson Reuters, number of articles published in the journals of *Nature* and *Science*, number of articles indexed in Science Citation

Index—Expanded and Social Sciences Citation Index, and per capita performance of a university. More than 1,200 universities are ranked by ARWU every year, and the top 500 are published. The University of Minnesota is ranked 30th overall.

Renee Frontiera

Professor Renee Frontiera received a prestigious National Science Foundation (NSF) CAREER program award. The Faculty Early Career Development (CAREER) Program supports junior faculty members who exemplify the role of teacher-scholars through outstanding research, excellent education, and the integration of education and research. With the CAREER award, Frontiera will develop and utilize a microscopic imaging technique capable of probing chemical structure on nanometer length scales, which should be applicable in a number of areas such as biomedicine, pharmaceutical and food safety, photovoltaic and photocatalytic device characterization, and materials science.

Wayne Gladfelter

Throughout his 36-year career, **Professor Wayne Gladfelter** has assembled a remarkable record of service to the Department of Chemistry, the College of Science & Engineering (CSE), the University of Minnesota, and to the discipline of chemistry beyond the university. In recognition of his outstanding service to the University of Minnesota and others, he was awarded the *2015 George W. Taylor Award of Distinguished Service* by the CSE. At all levels, Gladfelter was lauded for his commitment to providing excellent leadership, including serving as chair of the Department of Chemistry and associate dean for the CSE, his willingness to accept challenging assignments, his acumen as a creative problem-solver, his calm demeanor, and his generosity of spirit.

Christy Haynes

Professor Christy Haynes received a *2015 Sara Evans Faculty Woman Scholar/Leader Award*, sponsored by the Office for Faculty and Academic Affairs and the Women’s Center. This award recognizes women faculty at the

University of Minnesota who have achieved significant national and international accomplishments and honors, and who contribute as leaders on campus.

Haynes was awarded the *2015 Advising and Mentoring Award by the Graduate and Professional Student Assembly*. This competitive award honors advisers who create a culture of mentorship by helping students set realistic expectations, providing opportunities for professional development and/or research, and overcoming personal and professional challenges.

Four co-founders of the Center for Sustainable Nanoparticles (CSN), including **Haynes**, were honored with a “*100 Inspiring Women in STEM*” award and featured in the September 2015 issue of *Insight into Diversity*. These leaders were lauded for creating a welcoming climate within the CSN that encourages open and regular discussions on bias and gender-based differences, networking, and confidence. The women were also honored for their contributions to their scientific fields, collectively publishing more than 400 papers, giving talks around the world on their science, and working on issues related to women in science, technology, engineering, and math fields.

Marc Hillmyer

Professor Marc Hillmyer was awarded a prestigious *McKnight Presidential Endowed Chair*. This is one of the university’s highest faculty awards, honoring Hillmyer for his distinguished research, education, and public engagement activities. He is only the second professor in the university’s College of Science and Engineering to receive this honor. Hillmyer has nearly 300-refereed publications to his credit. He has advised or co-advised 38 doctorate students and 55 post-doctoral fellows, and mentored more than 90 undergraduate students in his laboratory. He has attracted more than \$9 million in sponsored funding as a principal investigator or co-principal investigator. He also led the successful effort to secure \$20 million National Science Foundation-sponsored Center for Sustainable Polymers. He also was one of the founders of the popular Energy and U outreach program.

Thomas Hoye

Professor Thomas Hoye received the *2015 Ernest Guenther Award in the Chemistry of National Products* from the American Chemical Society, honored for his outstanding achievements in the analysis, structure elucidation, and chemical synthesis of natural products. Hoye's research encompasses the development of new synthetic methods, nuclear magnetic resonance-based strategies for determination of absolute and relative configurations, and pro-drug and block polymer-based nanoparticles for drug delivery. Members of his research group demonstrated that benzyne can generally and practically be formed merely by heating appropriate triyne precursors—the hexadehydro-Diels–Alder (HDDA) reaction.

Steven Kass

Professor Steven Kass is the recipient of the *L.I. Smith Professorship*, chosen for his record of scholarship, research, teaching, and service. This five-year endowed professorship is effective, January 1, 2016. He joined the faculty at the University of Minnesota in 1986. His research interests currently focus on hydrogen bond catalysis, Brønsted acids and bases, and anion molecular recognition. For many years, he carried out a variety of mass spectroscopic studies.

Timothy Lodge

Regents Professor Timothy Lodge received the *2015 Herman F. Mark Polymer Chemistry Award from the Polymer Chemistry Division* of the American Chemical Society (ACS). This award is the highest honor given by the ACS Division of Polymer Chemistry, awarded once every two years. Lodge was honored for his outstanding leadership and research in polymer science. He is one of the most productive, innovative, and influential polymer scientists in the world, focusing his research on the structure and dynamics of polymeric systems. He has published more than 300 papers and supervised more than 100 graduate students and post-doctoral fellows.

Lee Penn

Professor Lee Penn was named a *2015 American Chemistry Society (ACS) Fellow*, honored for her outstanding contributions and service to chemistry, science, the profession, and the ACS. She has a long record of service to the ACS community, recently serving in a number of leadership positions with the Division of Geochemistry. Penn is an advocate for diversity. She has a personal and professional commitment to improving the diversity of people studying and working in science, technology, engineering and math fields. She is the founding chair of the Chemistry Department's Diversity Committee and co-leads trainings focused on how scientists and engineers can serve as allies to students with diverse backgrounds.

Penn received the *2015 Horace T. Morse-University of Minnesota Alumni Association Award for Outstanding Contributions to Undergraduate Education*. This honor is awarded to exceptional candidates nominated in the quest to identify excellence in undergraduate education. Penn has been a professor and researcher in the Department of Chemistry since 2001. She has a passion for teaching at all levels, including outreach to K-12th grade teachers and students, for mentoring undergraduate students, and for advising graduate students and post-doctorate researchers. She has taught a breadth of courses, ranging from general chemistry, freshman and honors courses, to upper level courses on materials characterization and green chemistry. She also shares her expertise on nanotechnology and passion for cycling in freshman and honors seminars.

Valerie Pierre

Professor Valerie Pierre was selected for inclusion in the *ACS Select Virtual Issue* on Emerging Investigators in Bioinorganic, which was published online by American Chemical Society (ACS). ACS Editors selectively highlight emerging scientists whose research is leading the field in new and exciting directions and whose work has appeared in *Inorganic Chemistry*, *Journal of the American Chemical Society*, *ACS Chemical Neuroscience*, and *ACS Chemical Biology*.

William “Will” Pomerantz

Professor William “Will” Pomerantz received a *Kimmel Scholar Award* from the Sidney Kimmel Foundation for Cancer Research. The Kimmel Scholar Awards were created to advance the careers of gifted young scientists involved in cancer research. Pomerantz was chosen for demonstrating the greatest promise and innovation in his work. His lab was awarded the grant for studying epigenetic regulation in various cancer models by the transcription factor BPTF through small molecule inhibition.

Lawrence Que Jr.

Regents Professor Lawrence Que Jr. received the *Japan Society of Coordination Chemistry (JSCC) International Award*. This award is presented to a researcher who has contributed to the development of coordination chemistry through outstanding and pioneering works. A preeminent researcher, Que's lab focuses on the unique challenges associated with dioxygen activation by nonheme iron in biological systems. His research group combines biological methods and inorganic synthesis with a range of spectroscopic and kinetic techniques to investigate how iron can activate dioxygen to carry out metabolically important and chemically interesting reactions. His group's work concentrations include high-valent iron-oxo, bioinspired catalysis, and nonheme iron oxygenases.

Theresa Reineke

Professor Theresa M. Reineke was appointed to the *leadership team of the American Chemical Society (ACS) Division of Polymer Chemistry (POLY)*. She serves as publicity co-chair.

J. Ilja Siepmann

Professor Ilja Siepmann was named associate editor of *Journal of Chemical & Engineering Data*, which is a monthly journal devoted to the publication of data obtained from both experiment and computation, which are viewed as complementary. There are 10 American Chemical Society (ACS) editors at the University of Minnesota—the highest number of ACS editors at one academic/research institution.

Energy & U—new location & Theatre Department collaborative

Attracting more than 10,000 students every year.

Since its conception 10 years ago, the University of Minnesota's Energy and U show has grown in popularity. It has also continued to evolve while remaining centered on its messages about energy, and its primary purpose of getting elementary students excited about science and engineering.

A new collaborative partnership with the university's Department of Theatre Arts & Dance is opening the door to additional possibilities for the show, including a higher level of professionalism and space for more students to attend. Last May, Energy and U moved to the Whiting Proscenium Theatre at the Rarig Center, which can accommodate 400 students per show, about 100 more than what were able to see the show in the Smith Hall auditorium. In addition, theatre students, faculty, and staff members are helping the Energy and U professors polish their presentations, and are providing professional-level sound, lighting, and music support. The shows now include multiple large display screens to enhance visibility of the graphics used in the presentation.

"We are excited about the opportunities this collaborative offers us," said Chemistry Professor David Blank, Energy and U director. He credits Marcus Dilliard, Department of Theatre Arts & Dance chair, for his enthusiastic response to the show and his vision for enhanced scientific communications by combining the talents of the scientist presenters and theater professionals. Dilliard and William Healey, Rarig Center's design/tech coordinator, made it possible for Energy and U to have access to a theater team with expertise in stage management, staging, and sound and visual technical assistance.



Professor Christy Haynes lights up methane-infused bubbles, which is always popular with the audience.

Since this collaboration is in its beginning stages, the Energy and U show will primarily focus on some initial enhancements to the current show, and learning how to best take advantage of the space and collaboration to maximize the impact on students in the future. What won't change is getting elementary students excited about science and engineering. It will continue to focus on teaching students about the First Law of Thermodynamics, the scale of world energy use, and the significant energy challenges.

The high-energy show has numerous explosions and demonstrations that often involve student volunteers from the audience, flames, and rock music that gets everyone dancing.

The presenters are professors David Blank, Renee Frontiera, Christy Haynes, Marc Hillmyer, and Aaron Massari from the Department of Chemistry, and Cari Dutcher from Mechanical Engineering. In addition to creating and coordinating the demonstrations, Joe Franek, Department of Chemistry lecture demonstration director, is also a presenter, on stage for all of the shows.

"One of our primary goals, exciting the students about the idea of going to college and pursuing a career in science and engineering, is a top priority," said Blank.

To reach this goal, outreach to schools with underserved populations of students is a priority, including those with

high percentages of students of color and students receiving free or reduced-priced lunch, which is an indicator of poverty. This outreach includes invitations to all public, private and parochial elementary and middle schools, 3rd grade through 6th grade, in the seven country metro area. Last year, the average percentage of all the schools attending was 56 percent in both categories. Demand for the show is high and continues to increase rapidly.

Generous support from the University of Minnesota Materials Research Science and Engineering Center and the Center for Sustainable Polymers, Medtronic, and Schlumberger offset bus transportation costs for participating schools. Most schools would not be able to attend without this support. The show is also supported by the departments of Chemistry and Chemical Engineering and Materials Science, and the College of Science & Engineering.

The show's messages and the outreach are making a difference. "Thank you so much for the awesome opportunity to attend the Energy and U event today. My kids loved it," wrote one third grade teacher after a show. "I teach at a very high needs school on the west side of Saint Paul, and many of my students do not know people other than their teachers who have been to college. On

the way there, one of my 3rd grade students asked, 'Why are we going to a university? This isn't for us. I'm not going to go to college.' On the way out, she said, 'I want to be a chemist when I grow up!' Showing the kids that science has fun, real world applications is the first step in inspiring them. I am so happy that your team planted the seed that she should strive to work hard and do something great in her life."

Energy and U continues to expand, said Blank. "We are



Joe Franek, who creates the Energy and U demonstrations, sets a gummy bear on fire to demonstrate how our bodies convert food into energy.

continued on back cover

Andrew Johnson awarded Baxter's Young Investigator Award



Andrew Johnson

development of medical products that save and sustain patients' lives.

Andrew "Andy" R. Johnson has been selected as a 2015 Baxter Young Investigator in recognition of his research accomplishments. This award stimulates and rewards research that can be directly used for critical care therapies and the

Andy is entering his fifth year of graduate studies in the laboratory of Professor Erin E. Carlson in the Department of Chemistry. His research focuses on the development of new analytical and informatics tools in the study of natural products, a rich source of therapeutic agents. Specifically, he is incorporating mass spectrometry-based techniques to enable rapid characterization of unknown compounds without the need for time-intensive purification efforts, streamlining the drug discovery process.

Andy is currently focused on the incorporation of cutting-edge techniques to the structure elucidation process, namely ion mobility spectrometry, which provides information about the size and

shape of molecules. Molecular modeling assists in the interpretation of these experimental results and prioritization of candidate structures for further study.

Andy received his bachelor's degree in chemistry and biochemistry, cell and molecular biology from Drake University in 2011. During his undergraduate research under Professor Mark Vitha, Andy studied the fundamentals of chromatographic selectivity. He then entered the doctorate program at Indiana University in analytical chemistry, joined the lab of Erin Carlson and began work in natural products discovery. Andy relocated to the University of Minnesota with the Carlson Group.

in MEMORIAM

Professor Emeritus Raymond Dodson

Professor Emeritus Raymond M. Dodson died in Minneapolis on Sunday, July 12, four days after his 95th birthday. Dodson was born on July 8, 1920, in the coal mining town of West Hazelton, PA. Through scholarships, he attended Franklin and Marshall College in Lancaster, PA, earning his bachelor's degree in 1942. He earned his doctorate from Northwestern University in 1947. He first came to the University of Minnesota as an assistant professor in 1947, and was promoted to associate professor with tenure in 1951. He left the university to work as senior chemist and assistant director for chemical research at Chicago-based G.D. Searle and Company from 1951 to 1960. Dodson returned to the university in 1960, serving as a professor of organic chemistry until his retirement in 1983.

Dodson was an outstanding scientist, studying heterocycles, steroids, and sulfur compounds. While working with G.D. Searle, he invented some of the first oral contraceptives, and he

supervised the program that led to the first antiadosterene. He also worked on penicillin manufacturing and artificial sweeteners. His research work in industry and academia resulted in the publication of more than 90 papers, and more than 70 patents.

He was an outstanding mentor and teacher, training more than 31 doctorate students, more than 15 students seeking their master's degrees, and numerous post-doctoral researchers.

Dodson was an active faculty member while at the University of Minnesota, serving on many department- and college-level committees such as the Dean's Ad Hoc Committee on the Reorganization of Chemistry, multiple search committees, University Patent Committee, Advisory Committee on Promotion and Tenure, and Consultative and Appeals Committee.

After leaving the university, he taught at the Fort Hare University in the Ciskei, South



Africa for two years before traveling the world with his wife Liz.

He was a family man, enjoying 33 years of marriage with his second wife Liz and her four children, and proud of his four children. He was preceded in death by his eldest daughter, Karen Bloom. He is survived by his wife Liz Brenner Dodson; children Steven Dodson MD, Debra Garley, MD, Becky Johnson, RHIT, CDIP; stepchildren Robert Brenner, Scott Brenner, Mark Brenner, James Brenner; 12 grandchildren and 7 great-grandchildren.

2015 Donors

The Department of Chemistry thanks the many generous alumni, faculty, corporations, foundations, and friends listed below for their donations and commitments to support the Department of Chemistry, our faculty, and our students. We are grateful for your support.

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For more information on giving or alumni involvement opportunities, please visit our web page at www.chem.umn.edu, or contact Kathy Peters-Martell at kpeters@chem.umn.edu or 612-626-8282 in the College of Science & Engineering Dean's Office.

This list includes gifts made from January 1, 2015, to October 1, 2015. Gifts received after October 1, will be included in subsequent donor lists.

Alumna becomes director of NSF Chemistry Division

Alumna Angela K. Wilson will become the new director of the National Science Foundation's Chemistry Division in March 2016. She earned her doctorate in chemical physics from the University of Minnesota in 1995, under the tutelage of the late Professor Jan Almlöf. A computational chemist, Wilson is currently a Regents Professor of Chemistry and director of the Center for Advanced Scientific Computing and Modeling at the University of North Texas.



Angela Wilson

Wilson's honors include the Francis P. Garvan-John M. Olin Medal of the American Chemical Society, International Union of Pure and Applied Chemistry Distinguished Woman in Chemistry, National Science Foundation CAREER Award, Quantum Systems in Chemistry and Physics Promising Scientist Award of Centre de Mécanique Ondulatoire Appliquée, and Wiley International *Journal of Quantum Chemistry* Young Investigator Award. She is a Fellow of the American Chemical Society, American Physical Society, and American Association for the Advancement of Science, and is a National Associate of the U.S. National Academies.

She has served on the editorial boards or editorial advisory boards of *Scientific Reports*, *International Journal of Quantum Chemistry*, and *Journal of Physical Chemistry*. She served on the editorial board of *Computational and Theoretical Chemistry* before she became editor in 2014.

Her research interests include the development and understanding of ab initio and density functional theory methods and basis sets, prediction of thermochemical and spectroscopic properties from main group to heavy element species, catalysis, and energy and the environment. She will be moving her research laboratory to the University of Michigan in January 2016.

Gifts from alumni and friends invaluable to the Department of Chemistry

By Kathy Peters-Martell

The approach of year end is a time of reflection and thankfulness. I am most thankful for the opportunity to work with the Department of Chemistry—our amazing and dedicated faculty, talented and deserving students, and supportive and involved alumni. Each year, we have been able to help more students through awards from alumni-established scholarship and fellowship awards, participation in the mentor program, renovated teaching and study spaces, and so many other interactions that give them a broad and comprehensive educational experience.

The department deeply appreciates our alumni and friends who have established scholarship and fellowship funds to help students. One grateful student recipient captured the impact and importance of these awards in a thank you letter to the donor. He wrote, "This award is helping me (and my family) afford my college education. But, more importantly, this award means that someone believes in me and my future and that my education matters."

We are grateful to our donors who are giving of their time and using their philanthropic dollars to help students obtain an education, provide resources for our dedicated faculty, support the ground-breaking research, assist with building improvements, or donate unrestricted funding to allow the department to take advantage of opportunities to enhance the curriculum and learning environment

Thank you.

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.

Professor Henry Albert Bent



Henry Albert Bent, a former professor of inorganic chemistry at the University of Minnesota, died in Pittsburgh on Saturday, January 3, 2015, at the age of 88. He was born

on Dec. 21, 1926, in Cambridge, MA, and was educated at the University of Missouri, Oberlin College (Bachelor of Arts degree, 1949), and the University of California at Berkeley (doctorate in physical chemistry, 1952). During World War II, he served as a radar technician in the U.S. Navy.

Bent was a professor of physical chemistry at the University of Connecticut and North Carolina State University, professor of inorganic chemistry at the University of Minnesota from 1958-1969, and director of the University of Pittsburgh's Van Outreach Program for taking demonstration-experiments to students throughout the Pittsburgh area. He wrote,

The Second Law: An Introduction to Classical and Statistical Thermodynamics (Oxford 1966), a book on Periodic Law and one titled, *Molecules and the Chemical Bond*. He also developed "Bent's Rule" on hybridization and valence bond structures. He was the recipient of several leading awards in chemical education, and was a popular lecturer on topics ranging from flames and explosions to science and abstract art.

His long career in chemistry culminated in unconventional ideas such as helium's placement over beryllium in the periodic table, the use of valence sphere models to create electron density profiles in molecules, and teaching through demonstration-experiments.

Bent is survived by his wife of 55 years, Anne; daughter Libby Weberg of Duluth MN; four grandchildren, Rachel and Drew Bent, and Kirsten and Alex Weberg. He was preceded in death by his son Brian, a chemistry professor at Columbia University.

in MEMORIAM

Department of Chemistry



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2,000 years
on a single-processor computer is equivalent to what supercomputer Mira—with 800,000 processors—can run in **1 day**

14 BILLION
gallons of ethanol were produced in the United States in 2014

40%
of corn grown in the United States is used to produce ethanol

19 gallons
of gasoline and **12 gallons** of diesel fuel are produced from one barrel of crude oil

USING ONE OF THE WORLD'S LARGEST SUPERCOMPUTERS, WE'RE MAKING DISCOVERIES THAT COULD BE HUGE FOR THE FUEL INDUSTRIES.

Producing fuel economically is a big challenge. The key is finding the best materials to convert chemical compounds. Researchers in the University of Minnesota's Department of Chemistry and the Department of Chemical Engineering and Materials Science are using a supercomputer at Argonne National Laboratory to discover materials that could improve the production of ethanol and petroleum products. It's one more way the future is being Made in Minnesota.



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Energy & U

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Professor David Blank, Energy and U co-creator and director, explains how a joule, equal to dropping a baseball about a meter, is the unit of measurement for energy.

excited about this opportunity to team with the Theatre Arts and Dance Department to enhance our presentations and communications efforts. By moving, more students will be able to see the show annually. But, more importantly, by working with the professionals in the theater department, we are taking this to the next level of engagement with those students, and showing them the possibilities that exist with the sciences and the arts.”