CATALYST

DEPARTMENT OF CHEMISTRY

Science. **At Its Source.**

Biannual Newsletter | Spring 2013 | THE UNIVERSITY OF UTAH®

Students in the computerized testing center in the Marriott Library generate data indicating which chemistry subjects students find most challenging

Cultivating Chemistry

Professor Charles Atwood makes the number crunching behind assessment analysis sound interesting. But that's what he does: Butch—as he likes to be called—makes it his business to turn abstractions into relatable concepts. Take IRT for example. "Item response theory," he explains, "unlike prior analysis methods, assigns an 'ability' to both the exam question and the student." In that distinction lies the ability of IRT to determine not only which test questions are the best discriminators of student capability, but also the topics that pose the biggest learning challenges. Professor Atwood's application of IRT methodology to a decade's worth of computerized test results showed which concepts University of Georgia chemistry students struggled with the most. That same approach has arrived, with Atwood, in Utah.

Professor Atwood is the first holder of the University of Utah's recently established Ragsdale Endowed Chair for Chemical Education. It's a position that offers significant flexibility to explore chemical education initiatives, and he's taking full advantage. Under his guidance, an IRT-based approach similar to that used in Georgia is being applied via a new 110-seat computerized testing center at the Marriott Library. Exams held

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Department of Chemistry

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there will generate the data needed to show which chemistry subjects today's undergraduates find most challenging.

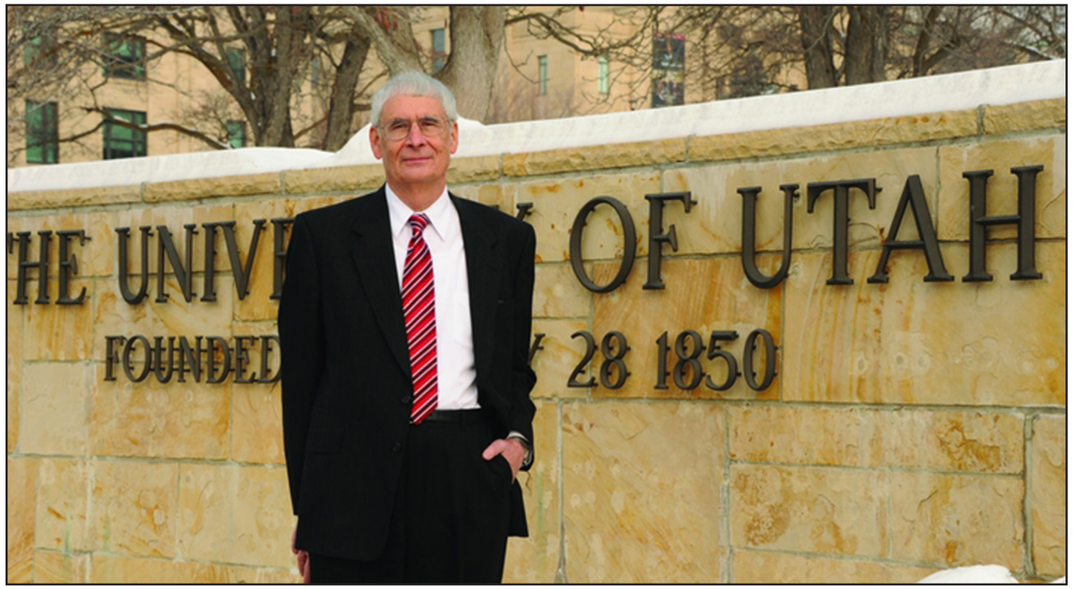
General chemistry is often thought of by students as a "weed-out" subject, a barrier to further study in the field unless one has a special knack. Atwood, and the Department of Chemistry, hope to change that notion, to *cultivate* students of chemistry by enhancing their ability to succeed in the classroom.

The benefits of IRT-informed chemistry evaluation may be significantly broader: the locally developed Canvas LMS (learning management system) offers a means to gather test data from high school chemistry students across the state. The aggregate data will identify the best test questions, but localized data will reveal topic-area weaknesses by district, giving individual schools the knowledge needed to focus teaching efforts and thereby boost performance.

In keeping with his interest in helping students achieve conceptual breakthroughs, Professor Atwood is engaged in other projects to promote a deeper understanding of chemistry. A study is under way to determine the effectiveness of metacognition, wherein learners think about their own cognitive processes and self-assess their progress. In another initiative, chemical demonstrations are being evaluated to see if they lead to the intended "Aha!" moments. Even more ambitiously, he hopes to deploy a technique developed in Sweden that provides a researcher with tactile feedback in the simulation of an enzyme with a substrate. Atwood wants to make that experience available to entire classrooms of chemistry students.

Imagine the collective "Aha!"

Story by Paul Bernard



Professor Peter J. Stang, Priestley Medalist, has led a research group at the University of Utah for nearly 45 years. Photo by Mitch Jacoby, ACS.

Prof. Peter Stang Captures Highest Award of ACS

The Priestley Medal, awarded annually by the American Chemical Society (ACS) for exceptional contributions to the field of Chemistry, was presented to Distinguished Professor Peter J. Stang at the Society's national meeting in New Orleans in April. Stang is former Chair of the Department of Chemistry, former Dean of the College of Science, and for the past dozen years, the Editor-in-Chief of ACS's top journal, The Journal of the American Chemical Society. Decorated last year by President Obama with the National Medal of Science, Stang is highly deserving of this recognition because of his pioneering research in molecular self-assembly and his monumental contributions to Chemistry at the University of Utah as well as nationally and internationally.

Outgoing chair Henry White and retiring Professor Ted Eyring both look pretty pleased to be leaving some of their long held duties behind.

Greetings from the Chair

Dear Alumni and Friends,

The past six months have been a tremendously active period for the Department of Chemistry. A fabulous dedication ceremony for the Thatcher Building for Biological and Biophysical Chemistry was held this past March, and we were pleased to see many alumni and friends at this event. The new building is fully occupied now by many research groups, and educational and outreach activities regularly fill the Reese Floor for Advance Undergraduate Laboratories and Curie Club Active Learning Center. The Thatcher Building will enhance the experience of generations of future undergraduate and graduate chemistry students and will be critical to the Department's research mission for many decades. We are extremely grateful to the support of alumni, friends, and corporations who helped make this wonderful new building a reality.

In this issue of the Catalyst, you will read stories about Prof. Ryan Steele's research in theoretical chemistry, and the work of Prof. Butch Atwood (the Ragsdale Endowed Chair of Chemical Education) to improve student learning in freshman-level General Chemistry. I am pleased to announce the recent establishment of the Thatcher Presidential Endowed Chair in Biological Chemistry. Presidential Endowed Chairs are rare at the University but are critical in attracting and retaining world-class researchers. They provide resources beyond conventional federal and state funding that allow chair holders to undertake high-potential, high-risk experiments. In addition to the new Thatcher Chair, the Department is particularly fortunate to have two additional Presidential Endowed Chairs: The Peter J. and Christine S. Stang Presidential Endowed Chair and the Henry Eyring Presidential Endowed Chair. Other news in the Catalyst includes Peter Stang receiving the Priestley Medal (the highest recognition of the American Chemical Society), the addition of two new assistant professors to the Department, and more. We are also sad to report the passing of our long-time colleague, Distinguished Professor David Grant.

It's been a great pleasure and honor to serve as the Department Chair during the past 6 years. We have a tremendous team of skilled staff and faculty who contribute so much to the Department's education and research missions. I am very pleased to announce that my successor is Distinguished Professor Cynthia J. Burrows, a long-time member of the faculty, and an exceptional chemist and educator. You can rest assured that Cindy will provide great leadership to the Department during her term as Chair.

On behalf of the faculty and staff in the Department of Chemistry, I hope this newsletter finds you well. Keep in touch and stop by next time you're on campus.

Warmest regards,

Henry S. White

Henry S. White
Distinguished Professor and Outgoing Chair

Curie Club Members Explore the Nano World

Mother/Daughter Event Brings Families Together in the Lab

Members and friends of the Curie Club teamed up with their kids and grandkids as lab partners for a nanochemistry experiment on April 26th.

Although nanoparticles are approximately 1/10000th the width of a human hair, the effect of converting dissolved $HAuCl_4$ in the presence of citric acid into gold nanoparticles is readily apparent when the heated solution turns nearly black and then deep red. Leading the workshop, Professor Jennifer Shumaker-Parry, whose research builds on the special optical properties of noble metal nanomaterials, explained that the deep red color results from the localized surface plasmon response of the gold nanoparticles. These properties can be harnessed for a variety of biomedical applications including detection of cancer or viral diseases.

The nanoparticles are stabilized as a colloidal dispersion by electrostatic interactions due to negatively charged citrate molecules adsorbed on the surfaces of the particles. The nanoparticles can act as sensors by exhibiting a color change from red to blue as the particles aggregate in different solution environments. As an example of this, participants added different reagents such as NaCl or sucrose to the nanoparticle solutions and watched for color changes.

Prof. Shumaker-Parry introduced examples of the use of colorful plasmonic metal nanoparticles from as long ago as the Roman period when the particles were used to colorize beautiful objects in glass. It was Michael Faraday who suggested that the size of the gold particles was key to the color, over 100 years ago.

The event was held in the C. Dale and Susan R. Poulter Laboratory adjacent to the Curie Club Active Learning Center in the new Thatcher Building for Biological and Biophysical Chemistry.

Rebecca Reese and her granddaughter prepare materials for the experiment.

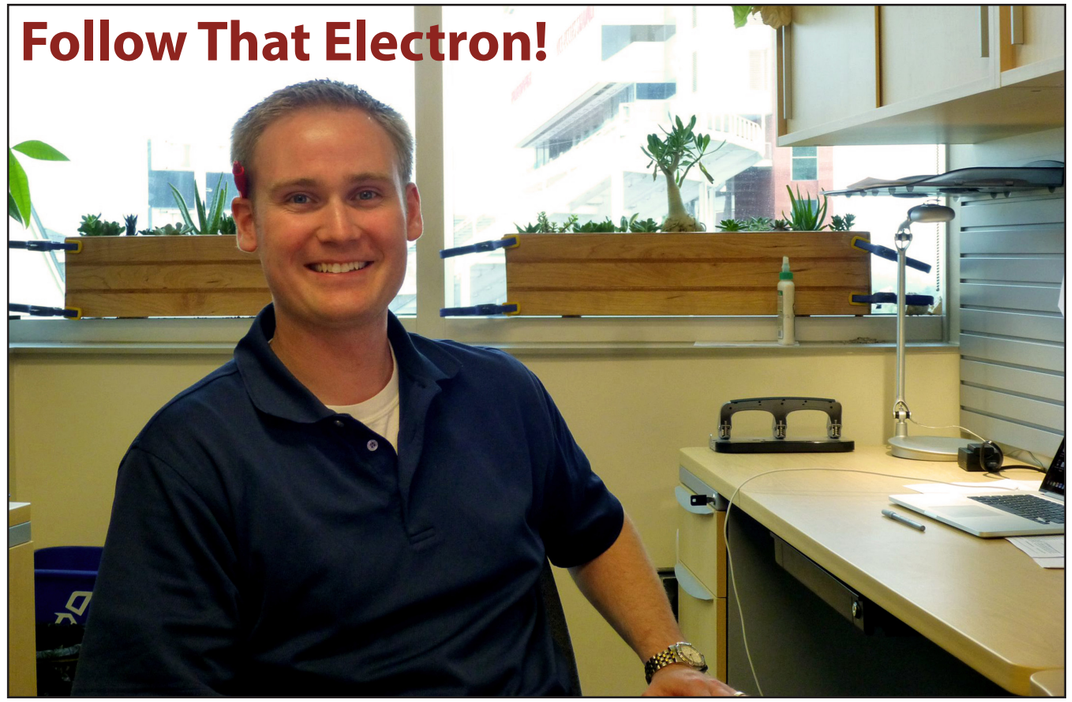
Anne and Ella Peterson listen to instructions from Prof. Shumaker-Parry.

One participant carefully transfers her solution to see the bright color.

Jennifer Sum and her daughter Katrina discuss the experiment.

Debbie Sigman and son Elias (left), and Deann Tilton and son Cruise (right) examine the results of adding Sprite to their sample.

Follow That Electron!

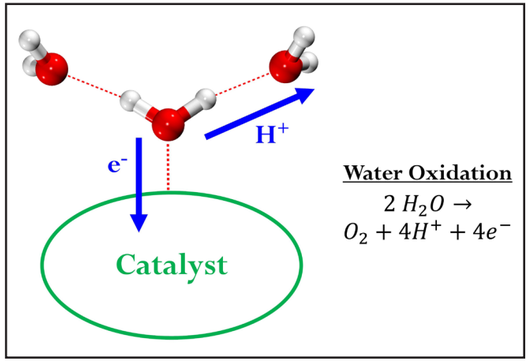


Professor Ryan Steele works in his office with his weekend project, planter boxes held together with sets of bar clamps.

Professor Ryan Steele points to the planters in his office windows, apologizing for their appearance. They look fine… except for the sets of bar clamps that are apparently keeping them from coming apart. "I made them over the weekend. Clearly, I'm a theorist," he says with a smile.

That's certainly true, though it's more aptly demonstrated by his quantum-chemistry simulations of water ionization. The approach, used by Steele and other members of the Henry Eyring Center for Theoretical Chemistry, recognizes the quantum mechanical nature of electron and light-nucleus interactions, wherein the wave nature of particles is dominant. The corresponding wave equations of these interactions, in all but the simplest cases, can't be solved exactly. But numerical methods, using new algorithms and faster computing resources—such as the University's Center for High-Performance Computing (CHPC)—are leading to ever more accurate simulations.

Such simulations are paving the way toward solar-driven catalytic splitting of water molecules, which can lead to large-scale production of hydrogen as a clean, renewable fuel. It's a tantalizing prospect: the Sun's energy splits water, yielding hydrogen. The hydrogen recombines with oxygen in a fuel cell, yielding just energy and water.



The initial step in splitting water: A solar catalyst enables loss of an electron, which drives proton transfer to neighboring molecules.

Still, supercomputers notwithstanding, identifying an optimum solar-catalytic sequence is no trivial task. That's underscored by some projected computation times: For one algorithmic approach, a detailed 20 picosecond simulation of a 17-water-molecule cluster is estimated to take 9 years. Using novel algorithmic methods, such as on-the-fly ab initio path-integral evaluation, Professor Steele and his colleagues aim to reduce that computational time dramatically. As the simulations improve, so will the chances of pinpointing which catalysts have the lowest cost and widest availability.

More broadly, the Henry Eyring Center, directed by Prof. Vale Molinero, is helping to shift the relationship between theory and experiment in chemistry. (When asked how the two camps interact, Steele responds, "Politely, of course.") Traditionally, theoretical chemists have been engaged with the explanation of experimental results. Increasingly, they're predicting what experimentalists will find. Beyond energy production, such an approach is profoundly impacting pharmaceutical research, where deeper understanding of drug chemistry can lead to molecular tweaks that improve drug efficacy… or to brand new therapies.

Professor Steele's interest in ionization also extends to a rather different effect: radiation damage in biomolecules. But in each area, the idea is to look past simple static structures and to understand how electrons and other ions drive chemistry. "If we know how electrons move, we know how molecules move," he says.

Story by Paul Bernard

Scholarship Honoring Prof. Edward M. Eyring Announced at Department Awards Ceremony

Each year, the Department of Chemistry recognizes our top undergraduates, graduate students, and faculty at the Department Awards Ceremony. On April 17th, over 55 awards and scholarships were given out to honor the hard work of 95 students and faculty. Dr. Craig V. Lee, Doctor of Dental Surgery, joined the program as the keynote speaker.

Additionally, our beloved colleague, Professor Edward Eyring, is retiring after more than 50 years of service as a member of the chemistry faculty. To honor his dedication and contributions to the Department and the world of chemistry, the annual Edward M. (Ted) Eyring Undergraduate Scholarship was established in his name as part of the Ragsdale Scholarship Endowment. As a unique component of these scholarships, recipients design, carry out, and report on a scholarly research project under the guidance of a chemistry faculty member. At the Department Awards Ceremony this spring, we named our first Edward M. Eyring Scholar, Levon Katsakhyan.

Many thanks to those who helped fund this scholarship including Michael and Vicky Farrow, Steve Kuznicki, Alberta Adsorbents, Jack and Margaret Simons, David and Diane Lentz, Steve Riseman, Charles and Dana Ebert, William McKenna and Ann Simonson, Melvin Miles, Joel and Frances Harris, and Henry White.

If you would like to make a contribution honoring Prof. Eyring, we are soliciting donations for a second scholarship in his name so that two students can be awarded this prize every year.

Levon Katsakhyan, the first Eyring Scholar, with Prof. Ted Eyring.

Doors Opened at Thatcher Building for Biological and Biophysical Chemistry in March

On March 13th, the Department of Chemistry dedicated the Thatcher Building for Biological and Biophysical Chemistry. The new facility, named in honor of the Lawrence E. and Helen F. Thatcher family, provides much-needed space for graduate research and undergraduate teaching laboratories.

The Thatcher Building is where our dedicated students will become distinguished scientists. The Department warmly thanks all the generous donors and supporters who made this a reality. It was a pleasure to celebrate the building's opening with all who could attend.

You can view more photographs from the Thatcher Building Dedication Ceremony and Ribbon Cutting online at http://giving.utah.edu/events/thatcher-building/.

Students volunteered to give tours of the new building to guests.

With his family watching, Lawrence Thatcher cuts the ceremonial ribbon in front of the Thatcher Building on March 13, 2013.

Waters Advanced Mass Spectrometry Lab to be Dedicated in September with Symposium

On September 20, 2013, the Department of Chemistry, in partnership with Waters Corporation, will hold a symposium on Innovations in Biological Mass Spectrometry. The event will also include a Dedication Ceremony for the new Waters Advanced Mass Spectrometry Laboratory, featuring the recently installed Waters Xevo G2-S QTof instrument.

The event will highlight diverse aspects of biological chemistry as revealed through mass spectrometry. Many distinguished researchers in the field will speak at the symposium, including Professors David Clemmer (Indiana University), Julie Leary (UC Davis), Joseph Loo (UCLA), John McLean (Vanderbilt University), Natalia Tretyakova (University of Minnesota), and Peter Armentrout (University of Utah).

Waters Corporation has generously donated the Waters Xevo G2-S QTof instrument for the new lab in the Thatcher Building. This instrument, worth over $500,000, ionizes chemical compounds to generate charged molecules or molecule fragments and measure their mass-to-charge ratios. It is designed to be adaptable with any future innovations in the field, ensuring the instrument remains current.

"Our partnership with Waters Corporation goes back over twenty years, and we are grateful for this recent gift," said Prof. Henry White, Department Chair. "The Department looks forward to Waters joining our conversations with leaders in mass spectrometry at the upcoming symposium at the University of Utah."

For over fifty years, Waters Corporation has designed, manufactured, sold and serviced mass spectrometry systems and other analytical instrumentation. Their work enables significant advancements in areas such as healthcare delivery, environmental management, food safety, and water quality worldwide.

The new Waters Xevo G2-S QTof instrument from Waters Corporation

Prof. Ryan Looper Wins Young Investigator Awards

University of Utah Professor Ryan Looper, whose research focuses on the behavior of small molecules within biological systems, is a recent recipient of Amgen's Young Investigator Award. The award, one of four such given annually by the biotechnology company, recognizes young scientists who demonstrate research excellence and make significant contributions to the field of organic chemistry and biotechnology that impact the practice of drug discovery.

As part of the award, Prof. Looper received an unrestricted research grant and was invited to give a lecture at the Amgen campus in Thousand Oaks, CA. The other investigators honored at the event were Sara Riesman (Caltech), Abigail Doyle, (Princeton), and Scott Snyder (Columbia).

In 2013 Looper was also recognized by Eli Lilly & Co., receiving one of only two nationwide Young Investigator Awards given by the pharmaceutical giant. This award is also accompanied by a major unrestricted research grant.

Using clues from nature, Prof. Looper's research group seeks to develop compounds as specific modulators of cell signaling events. More generally, they explore the mechanisms by which natural products behave in order to better understand the range of biological activities of these molecules. The research inspires the development of new potential drugs and synthetic methodologies.

News from the Department

Emeritus Professor David Morris Grant Passes Away

David Morris Grant, 82, died of natural causes on April 13, 2013 at his home in Salt Lake City, Utah.

Distinguished Professor Grant was former Chair of the Department of Chemistry and former Dean of the College of Science. He was a pioneer in the development of nuclear magnetic resonance (NMR) spectrometry. The David M. Grant NMR Center (also known as the Gauss Haus) was named in his honor in 2006. In his career, Prof. Grant received the Department of Chemistry's Distinguished Teaching Award, the Utah Governor's Medal for Science and Technology, the University's Distinguished Alumnus accolade, and the prestigious Rosenblatt Prize for Excellence.

Deslyn and David Grant

Though dedicated in professional, community and religious pursuits, Prof. David Grant will always be remembered for his devotion to family. His greatest fulfillment was in the lives of his five children, four step-children, forty-four grandchildren, and thirty-five great-grandchildren.

New Presidential Endowed Chair of Biological Chemistry

The Department of Chemistry is very excited to announce the *Thatcher Presidential Endowed Chair of Biological Chemistry.* The Thatcher Chair was established this spring by the generosity of the Lawrence E. Thatcher Family, for the purpose of supporting cutting-edge biological chemistry research in the new Thatcher Building for Biological and Biophysical Chemistry. The research laboratories of the Thatcher Chair will be permanently located in the Thatcher Building.

The $2.5 million Thatcher Chair endowment is a critically needed resource for the Department to attract and retain world-class chemists to the University of Utah. Graduate students and postdoctoral research associates supported by this gift will work in exciting new areas in biological chemistry related to the prevention and cure of human diseases. The endowment is especially valuable in providing means to undertake high-risk/high-potential experiments in testing transformative ideas.

Distinguished Professor and new Department Chair Cynthia J. Burrows is the inaugural holder of the Thatcher Presidential Endowed Chair of Biological Chemistry. Prof. Burrows is a world-class biological chemist, an outstanding educator, and a leader within the University and national chemistry community. Among her many research honors and awards, she is a member of the American Academy of Arts and Sciences, a Fellow of the American Chemical Society, and a recipient of the American Chemical Society Cope Scholar Award, one of the most prestigious research awards in the field of organic chemistry. She is an outstanding mentor and classroom teacher, receiving the University of Utah Distinguished Teaching Award and the Department's highest teaching honor, the Robert W. Parry Teaching Award.

The Thatcher Presidential Endowed Chair greatly enhances the Department's research and teaching missions as well as its academic ranking and prestige. The Department of Chemistry is very grateful for the support of Helen, Lawrence, and Tom Thatcher in making this Presidential Chair a reality!

Distinguished Professor Cindy Burrows (right) was caught by surprise when Tom (left) and Kathy Thatcher (center) announced she would be the inaugural Thatcher Presidential Endowed Chair of Biological Chemistry. Prof. Burrows has moved her lab into the new Thatcher Building's first floor.

2013 Distinguished Alumni Recognized in April

The Distinguished Alumni Awards recognize exceptional alumni from the Department of Chemistry. Our 2013 honorees are Richard D. Smith, George F. Uhlig, and Robert R. Webb. They were recognized at an awards dinner in April after presenting seminars on their work and dispensing advice to students.

Dr. Dick Smith completed his Ph.D. in physical chemistry under Jean Futrell in 1975. He is currently a Battelle Fellow, Director of Proteome Research, and Chief Scientist within the Biological Sciences Division of the Pacific Northwest National Laboratory. Dr. Smith's research centers on creating and applying new ultra-sensitive technologies to quantitatively probe entire proteomes expressed by cells, tissues, and organisms.

Dr. George Uhlig received his Ph.D. under Henry Eyring in 1972 while maintaining a career as a U.S. Air Force officer. He retired from the Air Force in 1983 at the rank of Lieutenant Colonel. Dr. Uhlig was employed by Hercules Aerospace until he began teaching college chemistry, first at Salt Lake Community College, then College of Eastern Utah. Dr. Uhlig retired from CEU in 2008 after founding the only science research program at the college.

Dr. Rob Webb completed his Ph.D. in 1982 as the second doctoral graduate of Gary Keck's lab. He entered the pharmaceutical industry with Bristol-Myers Squibb, where he worked on a variety of drugs to treat HIV/AIDS and cancer. Dr. Webb then moved to Arena Pharmaceuticals, where he helped develop the obesity treatment APD356 (Lorcaserin). He is currently Vice President at Amplyx Pharmaceuticals.

The Department is privileged to have such notable alumni and looks forward to recognizing a select few each year. To recommend an alumnus for this honor please contact Alyssa Geisler at ageisler@chem.utah.edu or 801-585-7896.

Dr. Webb addresses faculty and students in the Thatcher Seminar Room

Two New Faculty Members Join Department of Chemistry

We are pleased to announce two new faculty hires in the Department of Chemistry.

Dr. Matthew Kieber-Emmons will be joining the Department in August 2013 as an Assistant Professor. Dr. Kieber-Emmons is an inorganic chemist whose research interests are in designing new catalysts for chemical reactions that underpin energy related technologies (e.g., water oxidation from solar energy and oxygen reduction in fuel cells). Dr. Kieber-Emmons received his B.S. in Chemistry from St. Joseph's University (2002) and his Ph.D. in Chemistry from the University of Delaware (2008). He is currently an NIH postdoctoral fellow at Stanford University, working in the laboratory of Prof. Edward Solomon, where he has been combining spectroscopy measurements with theoretical calculations to develop a quantitative understanding of electronic structure contributions to chemical reactivity. Dr. Kieber-Emmons' research plans include design of transition metal catalysts for water splitting, spectroscopic studies of O-O bond cleavage in biological energy conversion, and a molecular-level mechanistic study of small molecule signaling in biology relevant to biotech development, biofuels, and food production.

Dr. Caroline Saouma will join the Department in January 2014 as an Assistant Professor and a member of the USTAR Alternative Energy Cluster. Dr. Saouma is also an inorganic chemist with research interests in the mechanism of small molecule activation. She received her B.S. in Chemistry at the Massachusetts Institute of Technology (2005) and her Ph.D. in Chemistry from the California Institute of Technology (2011). She is currently an NIH NRSA postdoctoral fellow at University of Washington, working in the laboratory of Prof. James Mayer, where she is studying proton coupled-electron transfer reactions using iron-sulfur clusters. Dr. Saouma recently received a prestigious American Chemical Society Division of Inorganic Chemistry Young Investigator Award. Her research plans focus on energy conversion strategies, including the development of chemical pathways for CO_2 fixation and reduction to methanol, and O_2 activation and reduction to H_2O (a major rate limitation of fuel cells). Her interest in the development of new technologies for the efficient conversion of energy is an excellent match to the objectives of the USTAR Alternative Energy Cluster.

We welcome Matt and Caroline to the Department!

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