

CATALYST

DEPARTMENT OF CHEMISTRY
Science. At Its Source.

Fall 2016 |  THE UNIVERSITY OF UTAH®



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GLOBAL CHEMISTRY

Dear Chemistry Friends and Alumni,

In this holiday season, we celebrate our connections across the globe. It's a time to remember former students, former colleagues, collaborators and friends, wherever in the world Chemistry may have led them since we last crossed paths at the U. We are a diverse bunch, we chemists—nearly a third of our faculty were born in other countries (Argentina, Austria, Hungary, Iran, Mexico, Panama, Russia, the UK and Vietnam), and one who I was sure hailed from overseas told me she was born in the U.S.A., but ethnically is a combination of Greek, Colombian and Lebanese! Our graduate student body is equally diverse with 30% of students coming from countries from Brazil to Sri Lanka, and most of the alphabet in-between. Our undergraduates are multilingual with considerable global experience as well. After passing through the hallowed halls of the Henry Eyring Building and the Thatcher Building for Biological and Biophysical Chemistry, our alumni move on to positions on many continents.

Global networking is made easy by the Internet, email, Facebook and other social media. We take these mechanisms for granted, and we think nothing of collaborating with scientists in different time zones—our colleagues are merely a Skype call away. This wasn't always the case, nor is it true for millions of Americans whose lives center on their hometown. It's a special bubble we live in, but one that encompasses the entire planet.

In October, three of us from Utah Chemistry spent a week in China (see photo of Profs. Scott Anderson, Peter Stang, and myself) speaking at the ACS – ICCAS Symposium on *Innovations in Molecular Science* in Beijing and also participating in the 60th Anniversary of

the Institute of Chemistry of the Chinese Academy of Science (ICCAS), with whom President Pershing signed a formal collaborative agreement last year. A week in China reminded me of how small the world is when everyone speaks the global language of Chemistry, and yet how diverse our cultures and cuisines can be. Certainly this diversity spurs us to higher levels of creativity and scholarship in our goals of education and research.

In this issue of *Catalyst*, we reach out to our alumni and friends, wherever you are. Enjoy the news, remember that your pathway brought you to the U, and please make the journey (virtual or real) back to us.

With best wishes for the New Year!

Cynthia J. Burrows
Distinguished Professor and Department Chair
Thatcher Presidential Endowed Chair of Biological Chemistry

RECENT FACULTY AWARDS

Scott Anderson	2016 ACS Award in Experimental Physical Chemistry
Bethany Buck-Koehntop	Career Services Faculty Recognition Award Celebrate U: Extraordinary Faculty Achievement
Joel Harris	2015 Governor's Medal for Science and Technology
Jennifer Heemstra	NSF Career Award W. W. Epstein Outstanding Educator Award
John Heemstra	Early Career Teaching Award
Valeria Molinero	Celebrate U: Extraordinary Faculty Achievement
Holly Sebahar	Career Services Faculty Recognition Award
Jennifer Shumaker-Parry	R.W. Parry Teaching Award
Matthew Sigman	Distinguished Professor
Jeff Statler	2016 Faculty Teaching Award for Excellence in General Education 2016 ASUU Student Choice Award
Ryan Steele	OpenEye Outstanding Junior Faculty Award in Computational Chemistry

CHEMISTRY BEYOND THE LAB

Computer Modeling with Valeria Molinero

Professor Valeria Molinero doesn't really remember how she first decided to study chemistry.

"When I was a child, I wanted to be an archaeologist, because I found it fascinating that in artifacts, you could discover the mysteries of the past." But then she started taking math classes, and she loved math. When she started taking physics classes, she loved physics. And when she started taking chemistry classes, she loved chemistry. By the time Molinero was starting college, her fascination had evolved to discovering how materials worked, not what they revealed about the past.

She completed her undergraduate and doctoral degrees at the University of Buenos Aires in Argentina, studying electrochemistry as an undergraduate, then statistical mechanics and computer simulations as a graduate student. She loved both of these areas of chemistry (surprise!).

"I actually like everything," Molinero joked.

When she moved to Caltech for a postdoctoral position, Molinero got a sense of how molecular simulations can be used to address more complex problems. Her first project was supported by Kellogg's. The goal was to use computer simulations to make crispier cornflakes. She also worked on modeling materials for fuel cell membranes.

A few years later, Molinero began her independent career at the University of Utah.

"I selected Utah for the amount of sun, I have to confess, and also because of the reputation of the chemistry department. But when I came for my interview, I really felt that it was a welcoming environment. The faculty, the people, the place are all wonderful."

Besides running her own outstanding research program, Molinero is the Director of the Henry

Eyring Center for Theoretical Chemistry. With collaborators in chemistry, biomedical informatics, medicinal chemistry, and materials science, the center is a space to study and discuss advances in the theory of molecular structure and interactions in these fields.

According to Professor Emeritus Jack Simons, the founder of the Henry Eyring Center for Theoretical Chemistry, theory is "a diverse field of chemistry that uses physics, mathematics and computers to help us understand molecular behavior, to simulate molecular phenomena, and to predict the properties of new molecules."

In computational chemistry, instead of working with real molecules, scientists like Molinero build mathematical models of molecules and their interactions.

"Computer simulations are a way of doing experiments, just within a computer," she explains. "The role of theoretical and computational chemistry is to provide more insight on how molecules interact and react. It's very similar to experiments, but cheaper. But they have to complement each other. You can only be sure that your model is right if you predict results of the experiment or you are able to validate with results of existing experiments."

Computational chemistry also allows the scientist to do things that might not be possible in a traditional lab. For example, you can look at what's called a "rare event." Let's say you have a glass of water, containing many moles of molecules. If you are looking for the behavior of just a few select molecules, it's very hard to find them. Computer simulations allow you to see something that is only a few nanometers in scale or happens in just a few nanoseconds. Simulations also enable you to design materials that do not yet exist, and then work with a collaborator to build promising materials.



"In some sense we are like the gods of the elements. We can go beyond what's accessible, and then other scientists can pick up our work and do something interesting from there," Molinero said.

Her project on fuel cell membranes is a good example of developing promising materials in models, then testing them with collaborators. The goals of this project are twofold: first, to develop and improve the methods used to model these materials; and second, to identify materials that have promising properties for the transport and the mechanical stability of the membranes.

Another interesting project that shows the diversity of Molinero's work has to do with understanding how water forms ice, particularly in cloud droplets. Clouds are made of droplets – these droplets nucleate around a particle that has the ability to absorb water such that it is going to favor the formation of a liquid particle. Most of these particles that are hydrophilic can produce a cloud droplet, but only about one in a million of the aerosols that exist in the atmosphere are able to induce the nucleation of ice. Scientists don't yet know what characteristics of the molecules induce the formation of ice, and this has been the focus of Molinero's group in the last few years.

"There are different temperatures at which ice can form, depending on how effective the surface is," she said. "We use molecular simulations, in which we build

models of the surfaces present in the atmosphere, to predict these temperatures."

The existence of water in the atmosphere, and what state it is in, controls Earth's energy budget, or the flow of incoming and outgoing energy in the Earth's climate system. When you have liquid water in the atmosphere, there is more absorption of radiation. When you have ice, there is more reflection of radiation. We can only predict the flow of this energy by knowing the temperatures at which different atmospheric aerosols can induce ice formation.

"This research is important for the accuracy of climate prediction models, which use set parameters for the density and type of aerosols," Molinero explains. "The more we understand how different types of aerosols form clouds and form ice, the better our climate predictions models will be."

What ties all of Molinero's diverse research together is her search to find simplicity in complex behavior.

"I like systems and questions that look complicated, but when you understand them, you see they are governed by a few rules," she said. "But to complete the picture you need a lot of people thinking, questioning your work, putting forward new hypotheses, and making mistakes that lead to new discoveries. I need the diversity of thinking of my undergraduate students, graduate students, and postdocs. The people who challenge and build on your ideas make science great."

NEW ENDOWED LECTURESHIPS HIGHLIGHT TEACHER-STUDENT RELATIONSHIP

A recent gift to the Department of Chemistry has established a unique pair of endowed lectureships. George and Camilla Smith, generous long-time supporters of the University of Utah, funded the Henry Eyring Lectureship in Chemistry and the Bryant A. Miner Lectureship in Chemistry in 2016.

These endowments memorialize two important chemists in the Department's history: Bryant A. Miner, Camilla Smith's brother, who earned his PhD in chemistry at the U in 1965 and taught countless chemists in his 43 years at Weber State University; and Henry Eyring, Camilla and Bryant's uncle, who established the U's Graduate School and was one of our nation's most renowned chemists.

These lectures are unique because of Henry Eyring and Bryant Miner's teacher-student or mentor-mentee relationship. Eyring was the thesis advisor for his nephew's doctoral degree. The inaugural lectures will be held in tandem, featuring two outstanding chemists who have the same mentor-mentee relationship. To our knowledge, there is

not any other program on campus with the same emphasis on this essential academic relationship.

The Smiths' generosity is not only a wonderful way to recognize Camilla's uncle and brother, but also a lasting benefit to generations of future students. The Department of Chemistry's Ph.D. program is the largest at the University of Utah, with over 170 students. These scientists are engaged in challenging yet rewarding fundamental research and teaching, carrying on the legacy of Henry Eyring and the many doctoral graduates of the past 70 years, including Bryant Miner.

The inaugural Henry Eyring and Bryant A. Miner Lectureships are tentatively scheduled for March 27-28th, 2017. We invite our alumni and donors to attend. The Henry Eyring lecture will be presented by Nobel Laureate Prof. Robert Grubbs (Caltech), and the Bryant Miner lecturer will be his former graduate student and now professor, Dr. Melanie Sanford (U. Michigan). We are delighted to honor the legacy of Professors Eyring and Miner with these exemplary scientists as our inaugural lecturers.

Starting in the 1950s, Henry Eyring ran annual foot races against his research students. In this photo, MarLynn James is on the far left. Henry Eyring is running second from the left. Bryant Miner is winning the race in the center. The student on the right is unidentified.



TEA TIME WITH WOMEN IN STEM

This year, the Curie Club is pleased to present a new event series reaching out to undergraduate and graduate women students across STEM fields. Each month, two successful women in science or engineering careers in academia or industry give advice, offer mentorship, and talk about their personal career paths to a large group of female students. The first few events have been filled with students eager to ask questions about managing stress, attending graduate school, balancing work and personal lives, and supporting other women pursuing degrees in STEM fields. We look forward to continuing these important monthly conversations.

Spring 2017 Tea Series

January 11, 2017
2:00-3:00 pm

Jennifer Heemstra
Associate Professor
U Department of Chemistry
Organic and Biochemistry

Sylvia Torti
Dean of Honors College
University of Utah
Science and Humanities



February 1, 2017
5:30-6:30 pm

Carrie Kelly
Professor-Lecturer
U Department of Chemistry
AMES Instructor

Mary Ann White
Materials and
Process Chief Engineer
Orbital ATK



March 1, 2017
2:00-3:00 pm

Bethany Buck-Koehntop
Assistant Professor
U Department of Chemistry
Physical and Biochemistry

Pearl Sandick
Assistant Professor
U Dept of Physics and Astronomy
Particle Physics and Cosmology

April 5, 2017
12:00-1:00 pm

Luisa Whittaker-Brooks
Assistant Professor
U Department of Chemistry
Inorganic and Materials Chemistry

Alla Borisyuk
Associate Professor
U Department of Mathematics
Computational Neuroscience



Curie Club
Inspiring Women, Supporting Science

NEWS FROM THE DEPARTMENT

Department raising funds for lectureship honoring Ted Eyring

Professor Emeritus Ted Eyring is a prominent figure in the memories of chemistry alumni. Ted has been a pillar of the department for over 50 years, and visitors still hope to drop in on him in his office. Since his retirement in 2013, we still see him around the building on occasion, and happily report he is doing well.

To celebrate Ted's recent retirement, and the consideration he always gave to his students and colleagues, the Department is raising funds to endow the Edward M. Eyring Lectureship in Chemistry. The Eyring Lectureship will invite eminent physical chemists to present their latest research to our students and faculty at an annual lecture. We welcome your support.

Gifts and pledges can be made online to the Edward M. Eyring Lectureship in Chemistry at www.chem.utah.edu/community/donate.php.

Pledges of \$2,500 or more can be extended over a three-year pledge period. Corporate matching programs are a potential way to double the impact of your gift.

In addition, we are collecting memories and updates from Ted's former students and colleagues to pass along to him. Please write a short note to Ted and send it by mail to Department of Chemistry, 315 S 1400 E, Rm 2040, Salt Lake City, UT 84112.

Please join us in recognizing Ted's tireless dedication to teaching, research, and service at the University of Utah.



New Department logo designed by graduate student



After a department-wide design contest and over 200 votes, a new logo was selected to represent the Department of Chemistry. Congratulations to Eric Amerling, who is a graduate student in Luisa Whittaker-Brooks's group. This logo will be used to represent the department during recruitment and outreach events. New merchandise including t-shirts, mugs, and water bottles will also soon be available. Keep an eye out for how you can order your own chemistry gear in the next issue of *Catalyst*.

Undergraduate peer mentors help students find their place

This fall, the Department of Chemistry started a new undergraduate mentoring program. Incoming chemistry students are matched with advanced chemistry students to serve as mentors.

Research has shown that graduation and retention rates increase by creating a sense of belonging when students first arrive at their university. In the Department of Chemistry, peer mentoring groups are established in the chemistry undergraduate seminar course to ensure that students develop a community within the department early in their academic career at the U. At the end of the semester, students go on a campus-wide scavenger hunt to find all the campus resources available to them during their time at the U. Photos of students on this year's scavenger hunt are below.

Due to the amount of time, effort, creativity, and motivation that the student mentors put into this program, the department is raising funds to relieve financial stress and compensate mentors for their contribution to the department. If you are interested in donating to the mentoring program, please contact chemistry's academic advisor, Tascha Knowlton, at natascha.knowlton@utah.edu.



HIGH SCHOOL TEACHERS TAKE MASTERS RESEARCH EXPERIENCE BACK TO THE CLASSROOM

The Master of Science for Secondary School Teachers (MSSST) degree program in the College of Science provides a unique opportunity for practicing secondary school teachers to earn an MS degree in science teaching with a focus on developing science content knowledge rather than pedagogy. The program is directed by chemistry professor Tom Richmond.

In the past two years, more than forty degrees have been awarded in this cohort-based program which culminates in an authentic hands-on research experience. Even experienced teachers find they benefit from a return to the college classroom. However, their research lab placements alongside graduate and postdoctoral students allow teachers to experience the process of research and contribute to the discovery of new knowledge.

For example, Woods Cross High School chemistry teacher Janette Duffin learned both synthetic and analytical techniques in the course of her investigation of the reaction chemistry of normally unreactive fluorocarbons. In particular she developed a new catalytic method to activate the exceptionally strong carbon-fluorine bond in organic compounds under mild conditions. Her discoveries may lead to new synthetic methods to make medicinally important fluorinated molecules or breakdown highly fluorinated molecules which are environmentally persistent.

Teachers ultimately take the excitement of research back to their classrooms, enhancing public education in Utah.

“ *The MSSST program has given me tools to enhance my teaching, from developing new skills or learning new models and analogies to the actual process of doing research. The research project allowed me to experience the excitement of discovering something new in the field of chemistry. I have been able to share this excitement with my students. It also helps me be a better mentor to students as they design and carry out their own research projects.* ”

- Janette Duffin, MSSST '16



The Noble Friends of Chemistry

Our community continues to be incredibly generous and supportive of our programs and research. Thank you to the many individuals, families, businesses, and foundations that made gifts to the Department this past year (Nov. 2015-Nov. 2016).

Radon Level (\$1,000,000+ Lifetime Giving)

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Thank !

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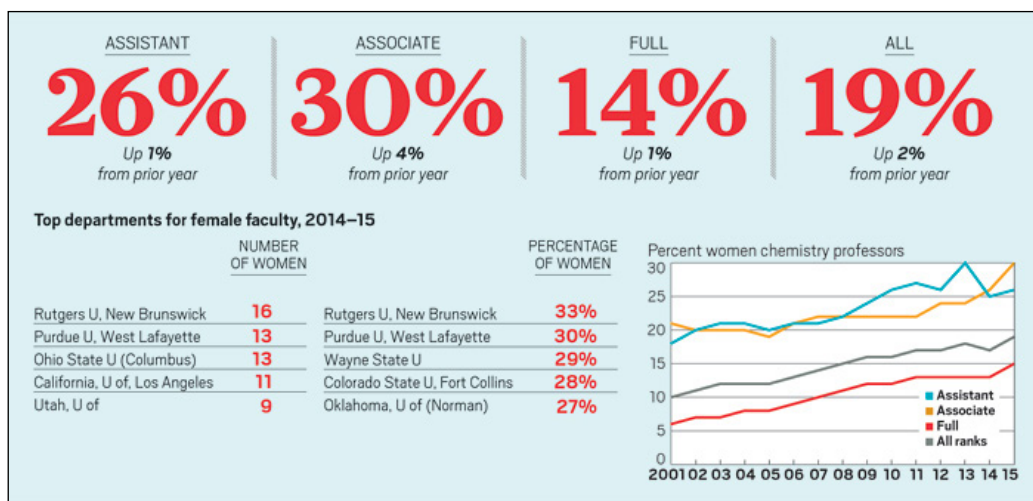
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The Department of Chemistry was recently recognized as one of the top departments for female faculty in *C&EN*. Of the top 50 schools in terms of chemical R&D spending, Utah comes in 5th in the number of women, and 6th for the percentage of women, at 26% - well above the average of 19%.

This data comes from the latest survey conducted by the Open Chemistry Collaborative in Diversity Equity (OXIDE), a diversity equity initiative cofunded by the National Science Foundation, the National Institutes of Health, and the Department of Energy.

Find more data and compare the 2014–15 stats with those that go back to 2011–12 at cenm.ag/oxide1213.

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