PURDUE UNIVERSITY

CHEMISTRY NEWS

PURDUE UNIVERSITY - DEPARTMENT OF CHEMISTRY

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Spencer Brown *(Photo of Paul Shepson taken on the frozen Arctic Ocean near Point Barrow, Alaska earlier this year. To learn more about Dr. Shepson's ozone research, visit the Purdue Chemistry web site to watch a video clip of the OBuoy project.)*

STAFF

MESSAGE FROM

DEPARTMENT HEAD

Dear Alumni and Friends,

We have just completed our academic year at Purdue and soon I will have completed my first year as Department Head. It has been a learning experience and adjustment for me personally. I have an active research group in the area of atmospheric chemistry and climate change, and I am working on improving my juggling skills. We have certainly had a busy year. One of my first objectives as department head was to hire a communications coordinator, Steve Scherer (scherer@purdue.edu), to better promote our Department, what we do and why it is important. Part of that strategy is reaching out to you—our alumni and friends. This is the first newsletter in what I hope will lead to a more frequent dialog and partnership with you.

Photo by Spencer Brown

What I consider as one of my most important tasks this year was the successful hiring of two new faculty members, especially in these difficult economic times. I am very pleased that Professor Mary Wirth will join our faculty as the W. Brooks Fortune Professor of Chemistry, and Dr. Yu Xia will join us as an Assistant Professor. These hires continue to bolster our strength in analytical chemistry and firmly place us as the world-wide leader in the field (This is our fully objective assessment!). We are also pleased that our faculty stands out, with a complement that includes approximately 30 percent women faculty members. This dovetails well with our newly developed departmental diversity plan.

This year has also led to a departmental commitment to focus on two important areas, drug discovery and energy development. We are focusing on these two areas as great opportunities for growth and impact. These interdisciplinary efforts are well-represented within our current faculty and will provide key partnerships with multiple departments on campus, as well as with industrial partners.

We are in the very early stages of aggressive development and planning for a new LEED certified facility that will serve as an energy efficient drug discovery and energy research laboratory and modern educational facility for our students. We promise to keep you informed as this exciting endeavor develops.

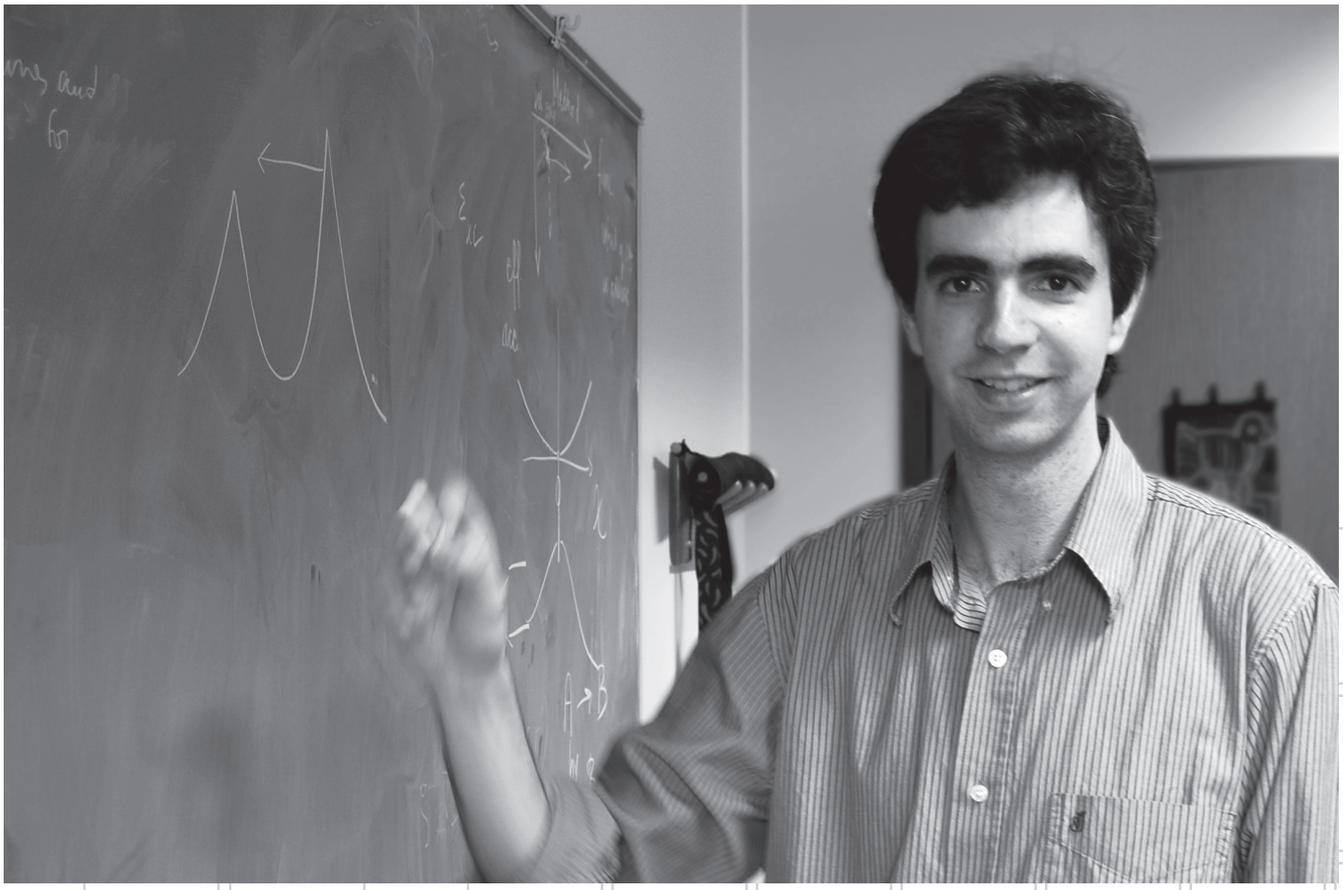
Over the course of the next year we have several key challenges ahead of us. We will adopt a departmental strategic plan, we will undertake a thorough review of our general chemistry and organic chemistry course offerings, and we will be enhancing our graduate student experiences. We will be welcoming a new Dean, Professor Jeffrey Roberts, who will also be a new faculty member in Chemistry. I look forward to getting him properly trained! It promises to be a challenging year ahead.

Finally, I invite you to share your ideas on how you believe we can better serve the needs of students and alumni, and improve the quality and impact of our Department.

Best wishes for the summer,

Paul Shepson

SCIENCE **FEATURE**



Professor Adam Wasserman

Goggles are not required when you visit the theory group. There are no wet labs, lasers, or mass spectrometers.

Instead, these scientists use imagination and mathematical analysis to calculate the behavior of atoms, molecules, and matter. "We try to explain chemical experiments using two tools—our brain and our computers," says Lyudmila Slipchenko, an assistant professor of physical and theoretical chemistry. Adam Wasserman, assistant professor of physical and theoretical chemistry, adds, "I don't get wet in the lab. My calculations are done in pencil and paper or on the computer. Of course there needs to be someone doing the experiments."

Both Purdue scientists stay up-to-date on the latest experimental research and also collaborate with colleagues. Slipchenko is working with Tim Zwier, M. G. Mellon Distinguished Professor of Physical Chemistry at Purdue, in analyzing the diphenylmethane molecule. "The idea is we can excite one part of the molecule and this electronic excitation transfers to other parts. A similar mechanism occurs in photosynthetic systems in biology," Professor Slipchenko said. This research has several energy applications including artificial photosynthesis and solar cell technology.

Professor Wasserman's goal is finding shortcuts to solve complex equations. He uses a popular technique called time-dependent density functional theory (TDDFT) to calculate excited states of molecules. "There

are many places for example, charged transfer excitations or double excitations, where density functional theory (DFT) fails. What I try to do is understand those cases where it fails, and try to figure out how to fix what is going on in those calculations," Wasserman explained.

Theoretical chemistry is a contemporary field and computing power advancement has played an important role in its growth during the past two decades. Walter Kohn and John Pople were awarded the Nobel Prize in Chemistry in 1998 for their work in ab initio and density functional theories. Wasserman noted, "Computers played a huge part in the development. It was in the 1980s when the main theoretical TDDFT foundations were established, but success in chemistry started only recently." "Anything we can't do with our brains, we teach the computers to do," explained Slipchenko. However there is more to theoretical chemistry than computers crunching numbers. "It is our job to then explain the phenomenon—make sure this is the result we expect and know why it happens," she said.

An additional area of Professor Slipchenko's research involves analyzing phase separation of alcohol-water-hydrocarbon mixtures in biofuel production. "Little is known about the molecular-level structure of the mixtures, but creating a robust, creative, and computationally-affordable theoretical model that can describe condensed phase processes will provide a major advance in better understanding fundamental interactions in liquids and solids," she said.

Professor Lyudmila Slipchenko

Professor Wasserman predicts a future where the computer will be able to tell scientists everything that happens in the experiment. "The dream is that one will be able to just draw a molecule on the computer screen—no matter how large—and just click a button. The program will calculate everything about that molecule—physical properties, excited states," he envisions.

$$i\hbar\frac{\partial\Psi}{\partial t}=\hat{H}\Psi$$

ALUMNI FEATURE

Dr. Thomas H. Lane *Peter Cutts Photography*

Dr. Thomas H. Lane is president of the American Chemical Society and a 1974 Purdue Chemistry undergraduate. He is a senior research scientist and director of global science and technology outreach at Dow Corning Corporation where he has been employed for the past 35 years.

You are at the halfway point of your presidency. As leader of the largest scientific society, what have been the unique experiences so far?

As president, I am the public face of chemistry – an awesome responsibility that I take extremely seriously. I have represented the discipline on "the Hill," at our national meetings, in the media, and in the colleges and universities around the world. Because of this role, I have had the opportunity to work and interact with hundreds of chemistry students and faculty from around the country. Native American, Hispanic, African-American, from coast to coast and everything in between. These students are extremely bright, full of energy and ready to take their place in chemistry – solving the global challenges that we face as a society. Coming from the chemical industry, I don't have the opportunity to work with students on a regular basis nor do I have the opportunity to see them in action. They are incredible!

I was especially excited and honored when the president of NOBCChE, Dr. Victor McCrary, presented me with a Kente Cloth at their national meeting in April. It was a tremendous honor for me and a visible statement of our commitment to work together for science and chemistry.

What advice do you give graduates seeking employment during the current economic climate? Does ACS offer resources for scientists seeking employment?

We are in very turbulent times but the economy will get better and the chemical industry will lead the way! I joined the work force in 1974 with the economy tanking, fuel prices out of control, and the economic outlook complicated by double digit inflation. However, competent chemists were still being hired.

Unemployment among chemists is still relatively low and great jobs are available today. They may not be exactly what a new graduate is looking for but there are great jobs available that will allow new employees to begin to shape their careers. Unlike the situation in 1974, we don't have to worry about the impact of inflation but, new graduates have to be more than just competent. Today's graduates must be the masters of the seven-C's! (www.thomaslane.org).

The ACS does offer a tremendous suite of products and services for members who are just starting out or who are ready to make a change in their careers. I would direct those interested in help to **www.acs.org/careers** for additional information. This site provides information for both job seekers and employers.

What is the future for American Ph.D. chemists in the chemical and pharmaceutical industries in this country?

First, let me say that I believe that this is the best time in history to be a chemist – a scientist. The problems facing this planet are huge and chemistry will play a central role in their mediation and in their ultimate solution. The global imperatives of clean water, food, alternative energy, a sustainable environment, and health care must be managed by our discipline and by our scientists if we are to survive. Remembering that anything you can see,

touch, taste, or smell is a chemical and therefore within our domain makes the future of chemistry and chemists look pretty good!

Now, regarding your specific question, I wish I had a crystal ball and I wish I knew exactly how the chemical enterprise will be organized in the future but, I don't. Clearly, the enterprise is changing. More chemists are working for smaller companies outside of the traditional market segments. There is a greater push for "greener" and for more sustainable solutions to our daily problems and that will certainly begin to change the way we work and how the industry is organized. Will the traditional bulk, specialty, and pharmaceutical chemicals ever go away? Not in my lifetime, but expect them to change size, direction, location, and agility. The industry is changing and that is a good thing.

Dr. Thomas H. Lane *Peter Cutts Photography*

How has your Purdue education influenced your chemical career?

I entered Purdue in 1970, the first in my family to ever attend college. I knew I wanted to be a chemist even though it was not clear to me what a chemist actually did for a living. I loved science and I loved the thought of solving problems that would help people. My high school chemistry teacher and a Purdue graduate, Kneeland Nesius (BS and MS Purdue) helped me find my passion for discovery and he not only believed in me, but truly inspired me.

I worked hard my freshman year at Purdue – I had a lot of catching up to do and I was working part-time to pay the bills. At the end of the academic year I was invited to participate in the honors chemistry program and my commitment to chemistry was solidified.

I had the incredible opportunity to work several semesters in research laboratories of both Professors Benkeser and Fuchs. Professor Benkeser was an organosilicon chemist and recipient of the Frederic Stanley Kipping Award in Silicon Chemistry sponsored by Dow Corning Corporation – he taught me how to work in a research laboratory – to be creative, he introduced me to silicon, and directed me to Dow Corning Corporation, a silicon-based company where I have enjoyed a 35-year research career.

My research experience with Professor Fuchs was equally rewarding. Prof. Fuchs allowed me to continue my interest in organosilicon chemistry and he made me a better chemist (competent). He taught me how to approach complicated problems and how to solve them, techniques and procedures that allowed me to be successful, the importance of effective communication and collaboration. These three men have had a tremendous influence on my life and my science.

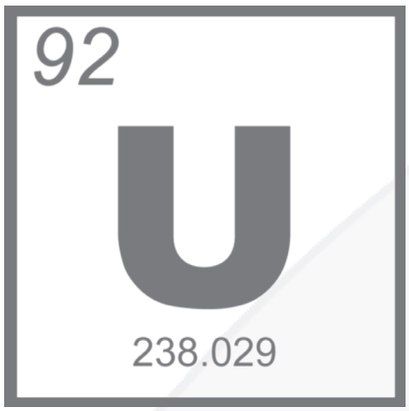
My time at Purdue was truly the best time of my life. My success in life is predicated upon the caring men and women of Purdue University who instilled my passion for learning and desire to help people. I have many wonderful memories of my time at Purdue – working in the kitchen at Wiley Hall, the endless hours in the chemistry building, and the tremendous friendships which made student life a blast!

I am proud to be a Purdue chemist; because the education I received provided me with the skills for improving people's lives through the transforming power of chemistry!

Editor's note: Purdue chemistry professor Joseph Francisco is ACS president-elect and will succeed Dr. Lane in 2010.

FACULTY FEATURE

Professor Suzanne Bart



Professor Suzanne Bart believes that uranium has a bad reputation. "There is a poor public perception that most people think it is just for blowing things up. But uranium has the potential to do many positive reactions as well, and unfortunately there is a general lack of understanding about these," says Bart.

Her research group is studying low-valent transition metals and uranium complexes for the activation of small molecules. "We are hoping that our research is going to move towards the way of catalysis. We are not currently doing catalytic reactions, but future energy applications where catalysis is required are a possibility," she said.

She decided to work with metals after taking an inorganic chemistry class in college. Bart later studied uranium during her post doctorate in Germany. "I think it is really fun chemistry because uranium is more reactive than transition metals. It's much more interesting because you can make unusual products and see more unexpected reactivity," she explained. "Some researchers don't want to work with uranium because of the radioactivity and the fact that the compounds are paramagnetic. Other researchers that study uranium also tend to be more interested in the coordination chemistry rather than the utility," Bart added. "But in our lab, we are excited to learn about the many uses uranium could potentially have."

Professor Suzanne Bart

Professor Bart is motivated by the potential of uranium as a catalyst and points out the history of the century-old Haber-Bosch process, which is used to make ammonia from its elements, nitrogen and hydrogen gas. Today Haber-Bosch plants produce enough ammonia to make about 500 million tons of artificial fertilizer a year. "Many people don't know that some of the first catalysts to perform this process were uranium catalysts. So uranium has the potential to do reactions that elements like iron and ruthenium do, which are currently used for making ammonia. I think that as scientists, we really don't understand the power of uranium because it has not been studied as much compared to these more well-known metals," she said.

Bart is adjusting to the routine of being a first-year, assistant professor of inorganic chemistry. She enjoys the variety of teaching, mentoring, and working on research projects in her new lab. "Unlike my post doctoral experience where I spent many hours in the lab, I now spend more time in my office working on lectures, problem sets, grading, reading the literature, and ordering equipment. So far it has been a very good experience," she says.

FACULTY AWARDS

Professor Hilkka Kenttämaa was presented the 2009 Provost's Award for Outstanding Graduate Faculty Mentor.

Professor Mark Lipton was selected as one of the top teachers of undergraduate majors in the College of Science.

Professor Christine Hrycyna was presented the department's Arthur Kelly Undergraduate Teaching Award.

Professor Dor Ben-Amotz was presented the College of Science Outstanding Undergraduate Teaching Award for class sizes up to 99 students.

The Purdue University Board of Trustees approved the appointments of Professor Arun Ghosh as distinguished professor of chemistry and medicinal chemistry and molecular pharmacology.

SPRING GRADUATES

UNDERGRADUATE DEGREES

Andrew W. Buesking
Ryan P. Davis
Michael D. Doud
Grace E. Kang
Allison O. Mattes
Elizabeth M. Roller
Sabrina R. Stone
Paul R. Warning
Kelsey G. Waters
Blake K. Williams
Nathanael R. Birt
Jonathan L. Bitner
Jeremiah D. Hammond
Alysia A. Lowe
Levi P. Sorg
Mark E. Stillman
David J. Windmiller
Matthew P. Fay
Patrick D. Haller
Mason R. Borlik
Christopher P. Colgan
Shakeel S. Dalal
Valerie R. Dooling
D. M. Griffith
Nicholas P. Ingram
Arisa Iwasaki
Kristen E. Klein
James E. Lancaster
Marc E. Willerth

ADVANCED DEGREES

Dr. Hongtao Chen (Analytical - Professor Cheng)
Dr. Shiyu Du (Physical - Professor Francisco)
Dr. Marc Fiddler (Analytical - Professor Shepson)
Mr. Pravin Gagare (Organic - Professor Ramachandran)
Mr. Michael Goodwin (Analytical - Professor Cooks)
Dr. Amy Griggs (Biochemistry - Professor Hrycyna)
Dr. Jamila Greene (Physical - Professor Francisco)
Dr. Hongling Han (Analytical - Professor McLuckey)
Dr. Sarah Hudon (Biochemistry - Professor Hrycyna)
Dr. Amanda Lee (Biochemistry - Professor Abu-Omar)
Dr. Marcela Nefliu (Analytical - Professor Cooks)
Ms. Nicole O'Neil (Organic - Professor Chmielewski)
Mr. George Pates (Analytical - Professor Kenttämaa)
Dr. John Slavin (Analytical - Professor Ivanisevic)
Dr. Ellen Steinmiller (Analytical - Professor Choi)
Ms. Jocelyn Tessman (Chem. Edu. - Professor Bodner)
Dr. Jun Xu (Analytical - Professor Skrynnikov)
Ms. Sonoeun Yem (Analytical - Professor Kenttämaa)

Interim Dean Jon Harbor (left) presented Frederick J. Palensky and John P. Longenecker with College of Science Distinguished Alumni Awards. Palensky (center) of St. Paul, Minn. is the executive vice president for research and development and chief technology officer for 3M. He received his doctorate from Purdue in 1977. Longenecker (right) of San Diego, Calif. is an executive in the biopharmaceutical industry. He earned his bachelor's degree from Purdue in 1969.

facebook

Reunite with classmates. Join the **Purdue Chemistry Alumni Group**!

IN MEMORIAM

William E. Truce, 91, professor emeritus of chemistry at Purdue died in January in Boulder, Colo. Professor Truce served on the faculty from 1946 to 1988. He was assistant dean of the graduate school from 1963 to 1969.

Shelton Bank, 76, died on Jan. 12 in Oakland, Ca. He earned a Ph.D. in chemistry at Purdue, studying under the Nobel Prize winner Dr. Herbert C. Brown. Bank was professor emeritus at SUNY Albany.

Joel E. Goldmacher, 71, died on Jan. 22 in Lakeland, Fla. Dr. Goldmacher earned a Ph.D. in organic chemistry at Purdue in 1963. He worked for RCA and founded Optel in Princeton, N.J.

Wilfred B. Howsmon Jr., 82, died on Oct. 8 in Sun City Center, Fla. Dr. Howsmon earned graduate degrees from Purdue in 1952 and 1955. He was the provost at the Manassas Campus of Northern Virginia Community College.

UPCOMING FALL DATES

Purdue Chemistry Alumni Luncheon
(Aug 17) 12-1:30pm
Walter E. Washington Convention Center
Room 209, Washington, DC
(Register through ACS - Event #909)

Distinguished Lecture Series:
The Purdue Lectures in Theoretical Chemistry - (Sep 23-24)

Outstanding Alumni Awards - (Sep 24)

Purdue 2009 Homecoming - (Oct 3)
Fooball: Purdue vs. Northwestern
Kickoff: Noon ET

Departmental Colloquium:
R.A. Walton Lecure - (Nov 12)

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Professor Joseph S. Francisco (center) visits with graduate students Robert Buszek (left) and Darryl Boyd (right) during Purdue's first annual NOBCChE symposium in spring 2009.