

Support Chemistry and CST

You can contribute to the continued success of CST and the Department of Chemistry by supporting scholarships, undergraduate research, faculty endowment and innovative programs. Make your gift at giving.temple.edu/givetocst.

CHEMISTRY

UPDATE SPRING/SUMMER 2017



Chair's message

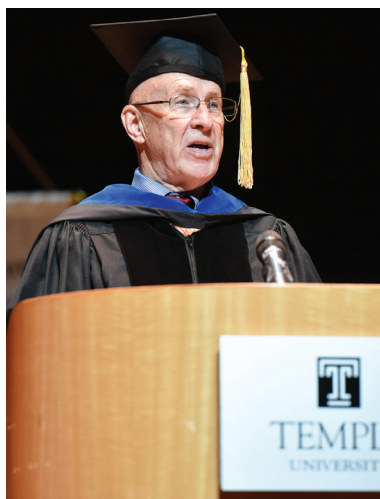
As we continue to build upon our teaching and research excellence, the Department of Chemistry owes much to faculty members such as Franklin A. Davis, Laura H. Carnell Professor of Chemistry, who retires in summer 2017. Since coming to Temple in 1995 as an already renowned organic chemist, Davis' contributions to the department's teaching and research growth have been profound.

Despite a difficult funding climate, the department's research excellence continues to grow unabated. Numerous grants this year to faculty from funding agencies such as the National Institutes of Health, National Science Foundation and Department of Energy have increased our annual research expenditures to approximately \$7 million.

This strong research infrastructure is supported by the enthusiasm and talents of our exceptional graduate student community. Just as I was writing this message, two of our graduate students won top awards for their research presentations at a Philadelphia American Chemical Society section event. Their work, in turn, is greatly complemented by our strong undergraduate researchers—many of whom, following graduation, go on to the country's finest graduate programs.

In short, the state of the department is excellent. Moreover, due to the strength and vision of our faculty and students, our continued ascent in both teaching and research will continue. Thank you to our alumni and friends whose financial contributions have contributed to our success. It is an honor to be able to take part in this academic mission with such a supportive chemistry community.

Daniel R. Strongin
Chair



Organic chemist Franklin A. Davis retires

The origin point of the Department of Chemistry's current momentum may have been the recruitment of Professor Franklin A. Davis, a distinguished organic chemist, from Drexel University in 1995. At that time, he was considering several offers, and while Temple had real advantages, there were also shortcomings.

"While the department had a high field NMR (nuclear magnetic resonance spectrometer), it lacked X-ray and mass spectrometry facilities and operational support for instrumentation," recalls Davis, who is retiring. "The laboratories were old and the heating and air conditioning were erratic."

During the past 22 years, he adds, "The department has continued to have wonderful support staff, but everything else has changed. Chemistry is now considered one of the top departments in the university."

The chemistry that Davis developed is regularly used by academic and industrial laboratories worldwide. His sulfur-nitrogen compounds (i.e., "Davis reagents") include N-sulfonyl oxaziridines for oxidations and asymmetric hydroxylations and N-sulfinyl imines (sulfinimines) for asymmetric synthesis of chiral amine derivatives. Among his honors are the Cope Scholar Award and John Scott Medal. He is a Fellow of the American Chemical Society and the Royal Society of Chemistry.

Last December, Davis delivered the College of Science and Technology's commencement address. "Beyond Frank's commitment to research, he always found time to be a tremendous mentor and supporter of students, assistant professors and colleagues in general," notes Daniel R. Strongin, professor and chair of the department. "The lively lunchtime conversations with Frank over the years will be missed by his colleagues. They added so much to the collegiality and vitality that define our department."

Davis says that he will not miss writing another proposal or even another paper. "What I will miss," he says, "are my colleagues and the many students I have had the honor and pleasure to teach and mentor over many years."

Matsika wins CST distinguished research award

Spiridoula Matsika, professor of theoretical/computational chemistry, is the most recent recipient of the College of Science and Technology Dean's Distinguished Award for Excellence in Research.

Her research, according to the 2016 award proclamation, "offers fundamental contributions to understanding conical intersections, the nonadiabatic dynamics of biological systems and laser control of molecular photodissociation."

Matsika's current funding sources include the National Science Foundation, for quantum chemical methods for studying photon- and electron-driven

processes in biological systems, and the U.S. Department of Energy, for combining high-level *ab initio* calculations with laser control of molecular dynamics of chemical and biological interest. The



latter represents a 10-year collaboration with Thomas Weinacht, professor at Stony Brook University in New York.

Says Matsika, whose work has recently been published in *Chemistry-A European Journal* and the *Journal of Physical Chemistry*.

"Overall, what I am interested in is trying to understand how molecules behave and react when they interact with light or electrons," says Matsika. "Another basic theme of my work, which is central to the NSF grant, is how light or radiation affects DNA, which may have applications for skin cancer."

Matsika is a fellow of the American Physical Society and has been an Alexander von Humboldt Fellow and a recipient of a prestigious NSF CAREER award. A native of Greece, she earned her PhD from The Ohio State University in 2000 and was a post-doctoral fellow at Johns Hopkins University before she joined CST in 2003.

"I love trying to understand how things work," she says, "and I also like the idea that the theory of quantum mechanics, which seems so abstract, can actually provide answers to real life problems and applications."

Chemistry helps launch CST post-baccalaureate pre-health program

The College of Science and Technology's Post-Baccalaureate Pre-Health Program has just completed its first highly successful year. Twenty-seven students—either college graduates who have not taken required science courses or those who want to burnish their academic science backgrounds—completed the program. According to Grace Hershman, associate vice dean and director of the CST post-baccalaureate program, 50 to 60 are expected in the second-year cohort.

Since 2008, faculty from the departments of Biology, Chemistry and Physics have taught the students in the Lewis Katz School of Medicine (LKSOM) Post-Baccalaureate Premedical Program. However, in response to a completely revised MCAT format in 2015, CST initiated a collaboration between these three departments to offer a completely customized pre-health, CST-based curriculum to those who do not necessarily want to limit themselves to LKSOM or to just medical school. The CST program also prepares students for admission to dental, podiatry, veterinary and physician assistant programs.

"It's a very challenging program with courses specifically tailored for students interested in going to medical school or other health programs," says Robert Rarig, who teaches an organic chemistry course for post-bacc students.

Theoretical chemist Nicholas Hestand will be a University of Chicago post-doc

Since his arrival at Temple in 2012, **Nicholas J. Hestand, CST '17**, who recently received his doctorate in theoretical chemistry, has been the lead author or co-author of 12 published papers.

"Some of my success has been due to hard work and some of it has been just luck, joining a fruitful project with Dr. Frank Spano," says Hestand, a Missouri native. "I can't imagine a better graduate experience. I've had a great advisor and great lab mates, and I've learned a lot about research."

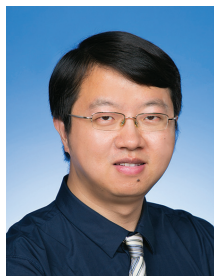
"Our research focuses on understanding the excited states of molecular aggregates and crystals, particularly in understanding what simple optical experiments, like absorption or photoluminescence, can tell us about a material's properties," says the recipient of both university and Francis H. Case fellowships. "For example, we've developed spectral signatures that allow us to predict whether a material would be good for transporting energy."

While commercial applications are beyond the research in which Hestand was involved, the basic principles of organic electronics that he and Spano's group have been exploring ultimately could have applications for generating solar electricity as well as television and smart phone screens.

Hestand will next be investigating water as a two-year post-doctoral fellow at the University of Chicago's Institute for Molecular Engineering.

"When I first came to Temple, my goal was to become a professor at a liberal arts institution where teaching would be my main focus, but during my time at Temple I've fallen in love with research," he says. "Now my goal is to find a faculty position where I can do both."





Bioorganic chemist joins faculty

Rongsheng (Ross) Wang is a new assistant professor in the Chemistry Department. Wang earned his PhD in bioorganic chemistry at Washington University in 2010. He worked at Mediomix LLC in St. Louis as a research scientist for two years following his graduation, where he was tasked with the development of antibody/aptamer-based homogenous fluorescent sensors and the invention of the novel SELEX platform for selecting aptamers. Wang left this position in 2012 to start a postdoctoral fellowship at the Scripps

Research Institute in San Diego. His work has been published in *Angewandte Chemie International Edition* and the *Journal of the American Chemical Society*.

Researchers explore new ways to detect and destroy chemical warfare agents

Department of Chemistry researchers have been awarded two different \$1.5 million grants from a U.S. Department of Defense agency for the exploration of new technologies that could be used to detect and destroy chemical warfare agents, toxic industrial chemicals and nerve gas. Each three-year grant from the Defense Threat Reduction Agency's (DTRA) Joint Science and Technology Office could also be extended another two years and funded an additional \$1 million.

Professor Eric Borguet is collaborating with a team of University of Pittsburgh researchers to develop more economical methods to sense and eliminate weapons of mass destruction. The researchers are investigating the use of what are called multifunctional, metal-organic frameworks (MOFs) with plasmonic cores comprised of metal nanoparticles.

"If we are successful in identifying metallic materials that are cheaper and more abundant than gold and silver, which are most commonly studied for these purposes," says Borguet, "it could impact not only chemical warfare agents but also other plasmonic applications."

Meanwhile, a Temple-led team that includes two Department of Chemistry faculty members, **Professor Christian Schafmeister** and **Associate Professor Michael Zdilla**, and researchers from UCLA and the Army Medical Research Institute of Chemical Defense (AMRICD) is exploring a new technology that has the potential to convert highly toxic organophosphate nerve agents into harmless phosphates.

The team plans to synthesize complex, shape-programmable macromolecules that are called "spirologomers" or "Molecule Lego." Much more robust and stable than currently used enzymes, Schafmeister says that these metal-containing macromolecules would be able to bind organophosphorus nerve agents and greatly speed up their breakdown into harmless compounds—and not generate immune responses in humans.

NEW RESEARCH GRANTS

Eric Borguet

- Design, Synthesis and Characterization of Hybrid Stratified MOF-Plasmonic Nanoparticle Materials for Detection and Destruction of Chemical Agents, *Defense Threat Reduction Agency*
- Electrical Properties of Single Molecules; from Switches towards Devices, *NSF*

Hai-Lung Dai

- Characterizing Interactions at Interfaces Critical to the Functions of Ionic Liquids and Solar Cells, *Air Force Office of Scientific Research*
- Nonlinear Light Scattering Spectroscopy and Microscopy of Molecular Interactions at Biological Surfaces, *NSF*

Graham Dobereiner

- Incorporating Lewis-Acid Anion CO-Catalysts into Homogeneous Transition-Metal Systems for Carbon-Carbon Bond Formation, *American Chemical Society Petroleum Research Fund*
- Tandem Catalytic Process in Flow, *American Chemical Society Green Chemistry Institute*

Robert Levis

- Detection of Explosive Signature Molecules Using Rotational Raman Spectroscopy, *Office of Naval Research*

Ronald Levy

- Computer Cluster for Computational Biology and Biology and Biophysics, *NIH*
- Computer Simulations of Protein Structure and Dynamics, *NIH*

Yi Rao

- Collaborative Research: Photoactivator Chemistry in Atmospheric Aerosols, *NSF*

Francis Spano

- DMREF-Collaborative Research: Developing Design Rules for Enhancing Mobility in Conjugated Polymers, *NSF*
- The Nature of Excitonic Coupling in Molecular and Polymeric Aggregates, *NSF*

Yugang Sun

- Microfluidic Synthesis of VO₂ Nanocrystals, *Argonne National Laboratory*

Vincent Voelz

- Markov State Model Approaches for Folding, Binding and Design, *NIH*

Sarah Wengryniuk

- Simplified Approaches to Medium-Sized Heterocycles for the Synthesis of Bioactive Small Molecules, *NIH*

Katherine Willets

- Plasmon-Mediated Electrochemical Reactions, *U.S. Department of Energy*

Michael Zdilla

- Exploration of Energetic Manganese Metal-Nitrogen-Oxygen Complexes and Clusters, *Office of Naval Research*

COLLEGE OF SCIENCE AND TECHNOLOGY

2016 DISTINGUISHED FACULTY AWARDS



The Dean's Distinguished Teaching Award

Ann Valentine, associate professor

The Dean's Distinguished Award for Excellence in Research

Spiridoula Matsika, professor

For more news, go to chem.cst.temple.edu

Kallie Willets honored at basketball game

Associate Professor Katherine Willets was honored for teaching and research during halftime of a Temple University men's basketball game. The February game against the University of Florida was also the occasion of CST's annual Hoops and Hoagies gathering for alumni and friends of the college. Willets earned her PhD at Stanford University and taught at the University of Texas, Austin before coming to Temple in 2015.



Chemical Society supports local students

The Temple University Chemical Society, a student group that works to improve science education in the local community, hosted the Setting the Spike for Science volleyball tournament. The event, which raised much-needed funds for science education at Cristo Rey Philadelphia High School, attracted more than 70 students, faculty and community members. More information about TUCS activities is available at tucs.weebly.com



Faculty Notes

George A. Petersson, Emeritus Professor of theoretical and computational chemistry and the Fisk Professor of Natural Science at Wesleyan University in Middletown, Connecticut, has been appointed distinguished adjunct professor.

Yugang Sun, associate professor, is the author and editor of *Nanomaterials for Photocatalytic Chemistry*, which the World Scientific Publishing Company published last November. The graduate-level and beyond book concentrates on the emerging area of the utilization of (solar) photon energy for catalyzing useful chemical reactions (also called artificial photosynthesis), including water splitting, C2 reduction, selective epoxidation, selective alcohol oxidation and coupling reactions.

David R. Dalton, professor emeritus of organic chemistry, is the author of *The Chemistry of Wine: Blossom to Beverage and Beyond*, which will be published later this year by the Oxford University Press.

Chemistry Department Reception at ACS in DC

Chemistry department faculty, alumni and friends will gather for a reception during the American Chemical Society's 254th National Meeting and Exposition in Washington, DC.

City Tap House
901 9th Street NW
Washington, DC 20001

Tuesday, August 22, 2017
5:30 p.m. to 7:30 p.m.

For details, contact
barbara.fles@temple.edu

