

From the Department Chair...

Greetings from the Department of Chemistry at MSU! Four years have passed since our last department newsletter and I sincerely hope this publication will give you a glimpse into today's department.



John McCracken

A recent headline in the Lansing newspaper announced unemployment in Michigan exceeding ten percent and continuing to be among the highest in the nation. While the economy is not news to anyone, the challenges of meeting the world's energy demands, solving problems in human health and providing the foundations for new industries presents many new opportunities for MSU chemists. Our department is addressing these issues through research and the preparation of the next generation of chemists.

In 2006, the state provided \$18 million to MSU for the purpose of constructing an addition to the Chemistry Building and renovating all of our undergraduate laboratory

classrooms. The addition is an extension to the front along Shaw Lane. Most of our classrooms and offices were moved into this addition in fall 2007. This move provided us 15,000 sq. ft. of space for research. We also moved all of the classroom laboratories used for organic chemistry to the west side of the first floor. These now feature advanced air handling and the capacity to meet our continued increase in science majors.

The new laboratory space also includes an NMR facility with three 300 MHz NMR spectrometers devoted to our undergraduate organic laboratory courses. Last spring, 751 students participated in organic chemistry lab courses and learned how to operate a modern, high-field NMR spectrometer. Plus, our advanced chemical synthesis course, CEM 415, now has the infrastructure needed to teach upper-class students the intricacies of preparing air-sensitive compounds.

Overall, the demand for chemistry classes has never been greater. The department issued 15,059 grades in our undergraduate courses for the 2007-2008 academic year.

Our faculty and their research students continue to prosper in the

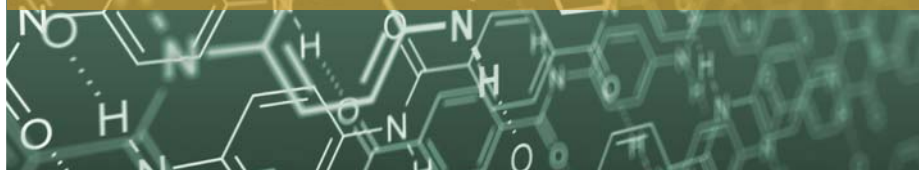
laboratory. Professors Smith, Maleczka and Dye (emeritus) were recipients of 2008 Presidential Green Chemistry Awards. Professor Piecuch organized and hosted the "13th International Workshop on Quantum Systems in Chemistry and Physics" and was elected as a Fellow of the American Physical Society last fall. As members of the National Superconducting Cyclotron Laboratory, Professors Bickley, Mantica and Morrissey played an important role in bringing the Department of Energy's \$550 million Facility for Rare Isotope Beams to MSU.

An exciting development in mass spectrometry has grown out of collaboration between Professors Dantus, Reid and Jones, and was recently featured in *Chemical and Engineering News*. Also receiving praise in the journal was the solid state NMR work of Professor Weliky pertaining to the chemical nature of proteins sequestered in bacterial inclusion bodies.

These are just several of our recent highlights. With 37 faculty and more than 200 advanced degree students involved in our department, there is not enough room for me to include updates on everyone. I invite you to stop by next time you find yourself on campus or visit the department's website to stay connected and join in the excitement that makes MSU a special place.

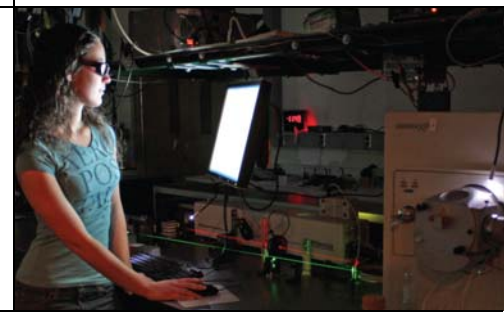
John L. McCracken
Chair, Department of Chemistry

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Advancing Proteomics with Ultra-Fast Laser Technology

For hundreds of years, dissection has been a useful technique for teaching human body functions as traditional blades cut apart tissue and organs to reveal the structure and function. Now, a new technique using a “laser scalpel” is advancing proteomics research by cutting apart molecules.



Christine Kalcic

Through an innovative approach of combining a mass spectrometer with an ultra-fast laser, MSU scientists studying proteomics are developing a technique for dissecting and examining the building blocks of individual cells.

Traditionally, mass spectrometry is used to break apart molecules and determine their composition. Molecules are ionized and then analyzed.

Graduate student Christine Kalcic is developing a laser that combines with the mass spectrometer so it can cut molecules more thoroughly and accurately than any methods currently available.

Kalcic began her third year in chemistry professor Marcos Dantus' lab this fall. She came to MSU from Harvey Mudd College in California, and has spent the last two years working on interfacing and instrumental work on the laser scalpel project.

This new instrument will allow users to tailor the energy that cuts apart ionized biomolecules. The Femtosecond Laser Induced Ionization/Dissociation method, or Fs-LID, will allow researchers to control

how molecules fragment and therefore enable them to learn more about the molecular structure and the biological systems that modify them.

The ability to break apart and analyze molecular compounds may lead to better medications, faster diagnosis of diseases and better treatments for illnesses, according to Kalcic.

“Getting one of the lasers to shine in the right spot of a commercially available mass spectrometer was actually pretty difficult,” Kalcic said. “Mass spectrometers are kept under vacuum so we had to get through all of the manifolds and electrodes and then weld and cap them with a view port for the laser to get in and out - all without compromising the vacuum.”

This new instrument is already being used for proteomics, metabolomics and lipidomics. Kalcic is studying a specific part of proteomics –posttranslational modification analysis.

“We are interested in post translation modification because it is a snapshot of a cell at a certain point in time,” Kalcic said. “If you took a sample when you were sleeping compared to a sample when you were running a marathon, the cells would be modified

differently; whether they are under oxidative stress, undergoing death or if they are cancerous.”

This new tool will provide a better understanding of protein synthesis and how the basic building blocks of cells change in response to stress. As the technology improves, it could be used to identify and diagnose illnesses and better understand how they operate on the cellular level.

The laser scalpel project is one of many ongoing ultra-fast laser research projects underway in the Dantus Lab. The lab group is also researching using lasers to detect chemical compounds remotely for use in bomb detection, selective photodynamic therapy to eliminate viral infections, laser control of single molecules and the development of new imaging and communication tools.

Coding New Methods in Quantum Mechanics

From his office in the Chemistry building, Jeff Gour uses quantum mechanical calculations to explain why molecules and nuclei behave the way they do. Gour is a doctoral student working under the guidance of Piotr Piecuch.

Since his arrival as an undergraduate in 2001, Gour has been an author or co-author on 26 published papers, and has received numerous awards and fellowships including the NSF Graduate Research Fellowship. He also received the Dallas J. Chapin Endowed Scholarship as an undergraduate. He earned his BS in chemical physics in 2005 from MSU.

His current research focuses on the development of new methods to do calculations of properties and energies of molecules. “We want to do quantum mechanical calculations on atoms and molecules,” Gour said. “So we develop new methods that are able to do that and produce accurate results while having computational costs that are affordable so that they can be used in a large number of applications.”

In the Piecuch Lab, researchers develop these methods theoretically, and then code them into computer

programs and distribute them around the world. These methods are used by scientists across all chemistry fields and provide the theoretical framework for understanding how basic interactions occur. A better understanding of this framework could lead to better energy sources, less damaging pollutants or any number of breakthroughs.

Gour attributes his early career success to his opportunities as an undergraduate. “My undergraduate research directed and set the pace for my graduate research,” he said. “I already knew what I was doing as my undergraduate research had already gotten my feet wet. I had shortened the learning curve so I could hit the ground running.”

He started doing research as a freshman in Mercuri Kanatzidis’ lab and by the summer of his junior year, he started working for Piecuch.



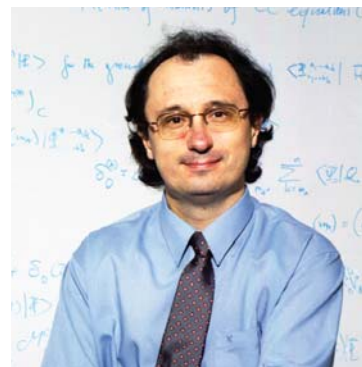
Jeff Gour

“That summer, I did research with him and I just continued from there,” Gour said. “I had a lot of success with my research and decided that I should stay here and continue my research at the graduate level.”

After he graduates from MSU, Gour plans to continue his work in methods development.

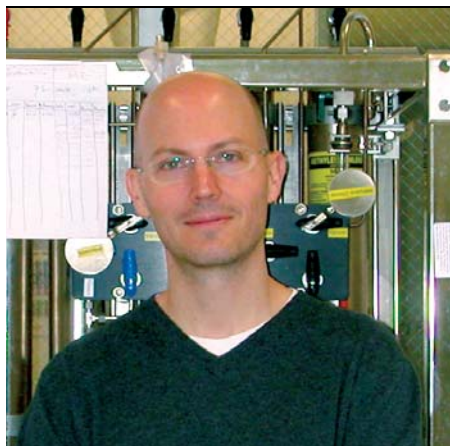
Piecuch Named Fellow of APS

Piotr Piecuch has been elected a Fellow of the American Physical Society for his contributions to electronic structure and quantum many-body theories, particularly developments in coupled-cluster theory and advances in understanding molecular properties, chemical reactivities, intermolecular interactions and nuclear structure. Piecuch is a University Distinguished Professor and an adjunct professor of physics. He earned a M.Sc. and Ph.D. from the University of Wroclaw in Poland. His research group designs and applies quantum-mechanical methods that enable precise determination of potential energy surfaces and property functions for both existing and hypothetical molecular systems in their ground and excited states.



Piotr Piecuch

Advancing Energy with Nano-Structures



Thomas Hamann received his B.A. in chemistry from the University of Texas, an M.S. from the University of Massachusetts and a Ph.D. from the California Institute of Technology in 2006.

Tom Hamann joined the MSU chemistry faculty this summer following his postdoctoral work at Northwestern University. His research interests in inorganic materials and electrochemistry of energy conversion and storage revolve around the theme of developing and characterizing nano-structured materials, coupled with detailed investigations of interfacial electron-transfer processes for solar energy conversion applications.

Hamann is also investigating controlling material composition and architecture at the nanometer length scale, understanding the surface/interface properties and tuning heterogeneous electron-transfer reaction kinetics to allow for rapid advances of the capture, conversion and storage of solar energy.

The efficiency of conventional planar photovoltaic devices is generally limited by the lifetime of charge carriers; efficient devices require pure and expensive materials. The development of nano-structured semiconductor

materials with controlled composition and geometry offers the potential for obtaining high-energy conversion efficiencies from more inexpensive semiconducting materials.

Hamann's work extends the generic concept of nano-structured photo-electrochemical cells to a wide range of materials, configurations and contacting phases. Advancement in this area relies upon increased understanding of interfacial electron-transfer reactions, interface stability and material structure and properties as well as the photoanode composition.

Two Faculty Receive NSF Career Grants

Two faculty members were recently awarded CAREER grants through the NSF. These grants support junior faculty who exemplify the role of teachers and scholars through the integration of education and research.

Kevin D. Walker received a \$700,000 award for his work studying molecular and biochemical evaluation of a phenylalanine aminomutase. He studies biosynthetic pathways of secondary metabolites that have potentially beneficial biological effects. The grant will assist in DNA informatics, biochemical analyses

and synthetic organic chemistry to better prepare students for careers in academia and industry.

Xuefei Huang received a \$400,000 award for his work studying carbohydrates and the role molecules play in processes such as inflammation, tumor metastasis, bacterial and viral infections. One of his successes is the syntheses of hyaluronan oligosaccharides as a biological probe. They play important roles in a wide range of biological events, such as tumor cell growth suppression, sensitization

of multi-drug resistant cancer cells, angiogenesis and immunostimulation.

With the support of the organic and macromolecular chemistry program, Huang plans to assay the sHA library obtained for their stimulatory activities toward toll-like receptor (TLR)-4, an important receptor involved in innate immunity. He plans to integrate students, postdoctoral researchers and high school students into his research while organizing outreach activities such as chemistry open houses and weekend science programs.

McHarris, Wagner Retire

Two long-time chemistry faculty and department icons to thousands of alumni have recently retired. William McHarris and Peter Wagner, Jr. have a combined 83 years in the department and have left a lasting impression on many alumni.

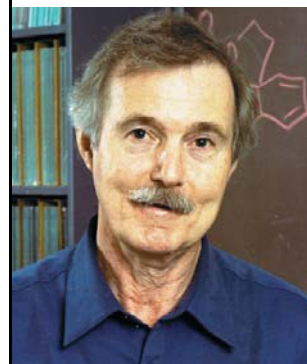
McHarris' career at MSU spanned five decades. He joined the faculty at MSU after receiving his B.S. from Oberlin College in 1959 and his Ph.D. from the University of California, Berkeley in 1965. His research concerned the structure and dynamics of atoms and molecules, and the development of quantitative descriptions for processes which occur at the submicroscopic level. His focus was on nuclear spectroscopy and reactions; exotic nuclei far from stability; mesons and nuclei, such as pion interactions/binding with nuclei; feedback from quark theory and elementary-particle physics into nuclear science and other fields.

Wagner also recently retired after a more than 40 years at MSU. He received his B.S. from Loyola in 1960 and his Ph.D. from Columbia University in 1963 before coming to MSU where he studied the chemical reactivity of photoexcited molecules.

Wagner mentored 47 graduate students and 19 postdocs, and with their help was able to publish 150 co-authored papers. One of his best-known papers was published in *Accounts of Chemical Research* in 1971 and was officially known as a "Citations Classic" because it has been cited more than 600 times.



William McHarris



Peter Wagner, Jr.

Chemistry Department Faculty Highlights

Abigail Bickley made significant progress with the design of an active target time projection chamber for use at the National Superconducting Cyclotron Laboratory at MSU. This device will be used to study reactions induced by short-lived nuclei at NSCL and at the future Facility for Rare Isotope Beams. The detector will be installed within a solenoidal magnet that was acquired from TRIUMF laboratory in Canada and was previously used as a medical MRI device.

Gary Blanchard graduated four PhDs in 2007! He has started a new collaboration with Frank Marken at the University of Bath focusing on the transport of molecular species across phase boundaries and is poised to move into the area of nanoporous solids.

Janice Hironaka teaches ISP207 for non-science majors and uses active learning activities, instructor-student interactions, and case studies. She is always looking for guest speakers to bring depth to the learning experience and asks interested alumni to email her at hironaka@chemistry.msu.edu.

Robert LaDuca leads an undergraduate-only research group investigating the synthesis and characterization of divalent metal dicarboxylate coordination polymers based on hydrogen-bonding capable tethering ligands.

Paul Mantica succeeded in measuring the beta-decay half-life of Sn-100. He continues to teach the freshman CEM 150 series and has been serving as National Director for the ACS/DOE sponsored Nuclear and Radiochemistry Summer Schools.

John McCracken continues as chair along with research and teaching. Shujuan Xu, a PhD student shared with Shelagh Ferguson-Miller in biochemistry, defended her doctoral thesis this past summer and submitted work to be published in the journal *Biochemistry*.

Greg Swain is involved in advanced carbon electrode development. The research targets dimensionally stable, high surface area electrocatalyst supports for fuel cells, and sensitive and stable microelectrodes for neuronal signaling in the gut and vasculature.

David Weliky was featured in the October 13, 2008 *Chemical & Engineering News* for a project in characterization of protein structure in bacterial inclusion bodies which are commonly formed during protein production for academic or pharmaceutical purposes.

EPA Green Chemistry Awards

The U.S. Environmental Protection Agency 2008 Presidential Green Chemistry Challenge Award recognized two MSU faculty members as well as a company affiliated with the department.



Milton Smith and Robert Maleczka

Chemistry professors Robert Maleczka and Milton Smith received the Academic Award for their work that resulted in a new environmentally friendly method for making complex compounds. Their discovery streamlined the manufacturing of chemical building blocks, eliminating the need for environment-threatening starting materials and significantly reducing the amounts of hazardous waste formerly associated with this process.

“Our technology makes the process more efficient and produces only hydrogen gas as the byproduct, so it is a win-win for companies to save money and reduce their impact on the environment,” Smith said.

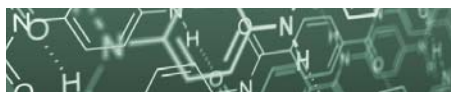
Smith recently patented a method for creating boron compounds which condense drug-making processes. Building off this, Smith and Maleczka received \$1.38 million through Michigan’s 21st

Century Job Fund to increase production of the patented chemical compounds and advance the research to the marketplace.

The EPA also recognized SiGNa Chemistry, Inc., with the Small Business Award. The director and founder of SiGNa is professor Jim Dye, and the company is actively involved with the department.

SiGNa received the award for developing a way to stabilize alkali metals while maintaining their usefulness in synthetic reactions. The stabilized materials are safer to work with and can also be useful in removing sulfur from fuels, storing hydrogen and remediating a variety of hazardous wastes.

Professors Karen Draths and John Frost previously received the Green Chemistry Award in 1998.



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Alumni Staying Connected

The department encourages all alumni to contribute information on accomplishments and special recognition in their careers for use in future communications. There are several ways for you to stay connected...

- Use the enclosed postage-paid envelope to mail us your news,
- Visit the Alumni section of chemistry.msu.edu and use the on-line form to send us your information,
- Join the MSU College of Natural Science group on Facebook or LinkedIn
- Join the alumni association and become involved in the college group.
- Visit the department website for the latest news on the department and for ways to stay involved: chemistry.msu.edu.

ALUMNI SPOTLIGHT:

Larry Dalton

B.S. Honors Chemistry '65

M.S. Physical Chemistry '66



Alumnus Transforms Communication Technology

Receiving the highest level of recognition from a national society is an extraordinary accomplishment. Alumnus Larry Dalton (Honors Chemistry '65, M.S. '66) has received three such honors and recently had an issue of the *Journal of Physical Chemistry* dedicated to him.

Dalton is credited with playing a critical role in transforming the research and understanding of organic molecules as the basis for solid-state optoelectronic and electronic technologies and opening up the potential of organic molecules for nonlinear optical applications. His lifetime of work has led to new device technologies, where ultrahigh bandwidth and low drive voltage devices are possible.

During his sophomore year at MSU, Dalton was working on a dual degree and became involved in undergraduate research with Professor Jim Dye. It was this research on pulsed radiolysis of the solvated electron that got Dalton engaged in research at Argonne National Lab and helped build a lifelong connection with Dye.

“Jim Dye changed our ideas of chemistry,” Dalton said. “It was MSU and Dye that gave me my scientific perspective and taught me how to approach difficult problems. I learned not to be afraid of any topic. Dye was an excellent teacher as he would lead

you through an understanding of the most difficult problems.”

Dalton credited Dye for his early success in density matrix theory and for sculpting his early career. Dalton's 610-page dissertation on electron-nuclear double resonance while at Harvard was the start of a productive career which currently includes 560 scientific publications.

Dalton is the B. Seymour Rabinovitch Chair Professor in Chemistry and the George B. Kauffman Professor of Chemistry & Electrical Engineering at the University of Washington. His early work on saturation transfer spectroscopy (including as a constant to Varian, Bruker and IBM) along with his latest breakthroughs on electro-optic materials have led to development of new materials and device concepts and to new companies. These breakthroughs have helped eliminate communication and computing bottlenecks and open new applications to improve defense, transportation and sensing technologies.

Photonic/electronic integration is Dalton's current challenge and research focus. “To continue to improve performance of computers



Larry Dalton

and other high technology components, we must create devices with incredible power efficiency as well as greater bandwidth (speed),” Dalton said. “These improvements in high technology require a rigorous, interdisciplinary approach. My approach to tackling difficult problems is that taught by Jim Dye. The approach is to be open-minded, fearless and interdisciplinary.”

Dalton has received the ACS Chemistry of Materials Award, the SPIE Lifetime Achievement Award, the IEEE Streifer Scientific Achievement Award, and the MSU Distinguished Alumni Award.

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Students Support Chemistry Day Event

Student groups in the department coordinated to celebrate National Chemistry Week in October with the 22nd annual Chemistry Day event. More than 1,200 people participated in the event at Impression 5 Science Center in Lansing.

The theme of the event was The Chemistry of Sports and demonstrations showcased the role of chemistry in sports and physical activities. Among the activities were the mechanics of throwing, determination of iron in cereal, polymers in sports equipment, the effects of density on floating, physical properties of ice relating to winter sports, and how different gases and temperature change the bouncing ability of balls.

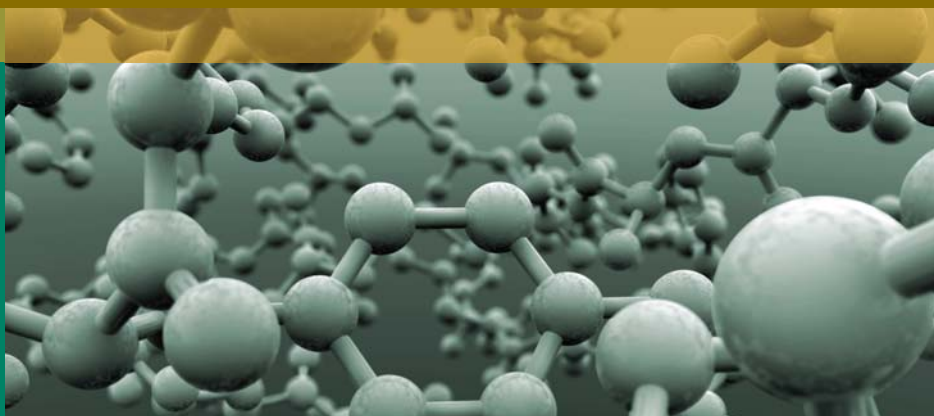
Activities and chemical demonstrations were presented by students from the department. MSU student organizations which participated included ACS Women in Chemistry, ACS Younger Chemists Committee, National Organization of Black Chemists and Chemical Engineers, Science Theatre, Alpha Chi Sigma and Omega Chi Epsilon.



Doctoral student Heather Pillman explains electrolytes and sports drinks to a Cub Scout during the annual Chemistry Day event at Impression 5 Science Center in Lansing. Photo by Xiaoyong Li.

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