

Greetings from the Chair

Welcome to the Fall 2012 issue of the Chemistry Department Newsletter. Despite a number of challenges, the past academic year proved to be another strong one for the Department, and the current academic year is off to a good start. Last year, the Department graduated 78 BSc., 9 MSc., and 24 PhD chemists. Currently, we have 254 declared chemistry majors in the undergraduate program and 215 students in the graduate program working toward their degrees.

Since 2006, the undergraduate population of the University has grown from 17,246 students to 18,427 students, and the number of chemistry majors has grown from 184 to 254. This growth means that the Department is providing 25% more course instruction for students, majors and nonmajors, and this has placed a significant burden on the faculty. To meet this growth the Department has worked to hire both tenure-stream and teaching faculty in an aggressive manner. Since 2006, twelve new tenure-stream and three teaching faculty have joined the Department. This year, the Department is pleased to welcome Professor Daniel Lambrecht (see page 11) who brings significant expertise in computational and quantum chemistry to the Department. While many of the faces in the Department may have changed since you last visited, the Department's philosophy remains centered on excellence in research and teaching.

The improvements to the buildings for the Chemistry complex and the Department's infrastructure continue. Since 2006, nearly five floors of the tower (14, 5, 4, 2, and parts of 10 and 3) and a floor of Eberly Hall (east wings of the 1st and 2nd floors) have been remodeled. In addition, the Annex above the Ashe Auditorium is fully operational, and this winter we will open the Chemistry Instrumentation Complex (CIC) to house the Department's NMR, Mass Spectrometry, and X-Ray crystallography resources in a newly remod-

eled space on the site of the former chemistry machine shop. In order to be more efficient and better serve researchers, the chemistry and physics machine shops and electronic shops have been combined, upgraded, and now operate as a resource for researchers throughout the Dietrich School of Arts and Sciences. The new joint machine shop is located in the NPL building (see page 14). While considerable renovation work remains (another 5 to 6 floors of the tower and parts of Eberly), the end goal is within sight and the rewards from the effort and investment are being felt already.

At the request of the Dietrich School of Arts & Sciences, the Department is engaging in a strategic planning process this academic year. The aim of this exercise is to reflect on the state of the Department and to identify strategies for improvement over the next five to ten years. Currently, we are in the stage of collecting information and data so that we can make informed decisions about future initiatives. As the process moves forward some of you may be solicited for your advice and input, and I hope that you will be generous with your time in helping us.

The stories in this newsletter highlight some of the people and events in the Department over the past year. I hope that these stories will provide you with some pleasurable reading and with a sense of the Department's life.

November, 2012



David H. Waldschmidt

Issue 9
 2012

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CALL FOR NOMINATIONS

The Department is soliciting nominations for the 2014 Chemistry Department Alumni Awards. Nominees should have a bachelor's, master's or doctoral degree from the Department. The basis for the nomination can be excellence in research, teaching, management, or volunteer efforts.

Nominations should include:

1. Your nominating letter
2. At least one but no more than three seconding letters
3. A CV for the nominee
4. Contact information for the nominee

Please see the alumni section of our Web page at <http://www.chem.pitt.edu> for more information

Nominations should be posted by December 1, 2013 to:
Assistant Chair
Dept. of Chemistry
University of Pittsburgh
Pittsburgh PA 15260

Alumni Award Celebration:

This year the Department recognized three outstanding alumni who have made important contributions in research and business for the betterment of science, the nation, and mankind.



Ben Askew received his Ph.D. in Chemistry from the University of Pittsburgh in 1988 under the direction of Professor Julius Rebek. Last year Ben joined the Boston-based VC firm Third Rock Ventures, LLC as an Entrepreneur-in-Residence where he provides expert guidance and scientific leadership to the VC firm and its portfolio companies. Ben also serves on the Board of Trustees at Gannon University, on the Scientific Advisory Board of Blueprint Medicines, and as a consultant for several Boston area biotechnology companies.

Rich Colton earned B.S. and Ph.D. degrees from the University of Pittsburgh, Department of Chemistry in 1972 and 1976, respectively. He performed graduate work under Professor J. Wayne Rabalais in ultraviolet and X-ray photoelectron spectroscopy. Rich is currently Head of the NRL Chemistry Division, having risen through the ranks from postdoc, to staff member, to Section Head and Branch Head, until his selection as Division Head in 2007. The Division conducts basic and applied research in chemical dynamics and diagnostics, materials chemistry, corrosion science and engineering, surface chemistry, and fire science.

Nadrian C. Seeman received his BS in biochemistry from the University of Chicago, and his Ph.D. in crystallography from the University of Pittsburgh in 1970. A member of the New York University faculty, Ned is widely recognized as a pioneer in nanoscience. When told in the mid-1980s that he was doing nanotechnology, his response was similar to that of M. Jourdain, the title character of Moliere's *Bourgeois Gentlehomme*, who was delighted to discover that he had been speaking prose all his life.



Left to right: N. John Cooper, Rich Colton, Alfred Moyé, Ben Askew, Jr., Costas G. Karakatsanis, Nadrian C. Seeman, David H. Waldeck and Dick Howe

Heroes of Chemistry Award given to Srikanth Venkatraman (Ph.D. 1996, Wipf)



Srikanth Venkatraman (Ph.D. 1996, Wipf) and his team at Merck & Co. are the recipients of a 2012 Heroes of Chemistry Award. They won the honor for developing the chronic hepatitis C drug Victrelis® (boceprevir). Victrelis® was the first oral hepatitis C virus protease inhibitor approved by the U.S. Food and Drug Administration. It is used in combination with pegylated interferon alfa and ribavirin to treat the most common type of chronic hepatitis C. Chronic hepatitis C is a viral infection that affects about 130-170 million people worldwide and can cause serious liver damage. Established in 1996, the ACS Heroes of Chemistry program recognizes scientists whose work in various fields of chemistry and chemical engineering has led to the successful innovation and development of commercial products that benefit humankind.

www.chem.pitt.edu



Chemistry Department History 4: Mellon Institute

The Chemistry Department's early research history was closely linked with the Mellon Institute of Industrial Research. Established in 1911 by Andrew W. and Richard B. Mellon, the Mellon Institute began as an industrial research department of the University of Pittsburgh and was incorporated as an independent non-profit entity in 1927. The Mellon Institute is recognized as the first major industrial research institute in the United States. Its original concept can be traced to Dr. Robert Kennedy Duncan, a Professor of Chemistry at Pitt from 1910 to 1914, who promoted an alliance between scientific research and industry that would encourage innovation in the discovery and development of new and improved materials, processes, and consumer products.

The first home for the Mellon Institute was in the building now known as Allen Hall (see photo) that was constructed at a cost of \$230,000 (ca. five to six million 2012 dollars) and was dedicated on February 26, 1915. It was not long before the Institute outgrew this facility, so a new building was constructed across from the Cathedral of Learning and the staff moved there in 1937. It remained an active and independent research institute until its merger with the Carnegie Institute of Technology in 1967.



Allen Hall



Mellon Institute

In 1913, the first Ph. D. degrees in Chemistry from the University of Pittsburgh were conferred on researchers from the Mellon Institute, and the relationship between the Department and the Mellon Institute continued for many years. One of the later Ph.D.s, Dr. Paul Lauterbur (Ph.D. 1962), went on to win the 2003 Nobel Prize in Medicine for his development of Magnetic Resonance Imaging. Lauterbur's idea of introducing gradients in the magnetic field for imaging applications had its foundations laid during his Ph.D. work at the Mellon Institute and the University of Pittsburgh. In the one hundred years since those 1913 Ph.D. awards, over 1300 men and women have earned their Ph.D. from the University of Pittsburgh, Department of Chemistry.

From its inception, Mellon Institute scientists studied chemistry, chemical engineering, biology, physics, and metallurgy because it was these disciplines that advanced the growth and prosperity of the Pittsburgh industrial empire. Today the Department's researchers carry on this tradition in a variety of ways, including the discovery and development of nanomaterials, chemical sensors, new methods for characterization, natural products, new therapeutic agents, new modeling and simulation algorithms, and biologically inspired polymeric systems; and always in the pursuit of a deeper understanding of nature from a chemical perspective. Continuing a proud heritage that started a century ago, the mission of the Department of Chemistry remains one of scientific discovery and innovation.

Faculty 1972

W. Edward Wallace, Chairman

Edward McCollin Arnett, Professor

Richard A. Butera, Assoc. Professor

James Clyde Carter, Assoc. Professor

Toby M. Chapman, Asst. Professor

Johannes Francois Coetzee, Professor

Theodore Cohen, Professor

Raymond S. Craig, Professor

Samuel J. Danishefsky, Professor

Kenneth E. Daugherty, Assoc. Professor

Bodie E. Douglas, Professor

Paul Dowd, Assoc. Professor

T.H. Dunkelberger, Professor and
Assoc. Dean, College of Arts and Sciences

Frank Oscar Ellison, Professor

Lawrence M. Epstein, Assoc. Professor

Henry S. Frank, Professor

Klaus H. Hofmann, Professor and
Director of Protein Research Lab

Charles Alvin Hollingsworth, Professor

George Allen Jeffrey, Professor

Kenneth Jeffrey Johnson, Asst. Professor

Frederick Kaufman, Professor

Robert Levine, Professor

Carolyn Wood Maricondi, Asst. Professor

Richard Hugh McCoy, Professor
Dean and Director of Graduate Programs,
Faculty of Arts and SciencesFoil A. Miller, Professor and
Director, Spectroscopy Laboratory

Alfred Leon Moyé, Asst. Professor

David Wixon Pratt, Asst. Professor

V. Udaya Shankar Rao, Asst. Professor

Jerome L. Rosenberg, Professor and Dean
of Faculty of Arts and Sciences

Hurd Winter Safford, Professor

Peter Emil Siska, Asst. Professor

Darel K. Straub, Assoc. Professor

Joseph J. Taber, Assoc. Professor

William Edward Wallace, Professor and
Chair

Robert L. Wolke, Professor

Class of 1972: Where are they now?

In 1972, we could fill a 20 gallon gas tank for \$11, but the average annual income in the U.S. was \$11,800, and the Dow Jones hit a new high at 1000. Hewlett-Packard introduced the HP-35 handheld calculator at a cost of \$395. In the news, U.S. ground troops were withdrawn from Vietnam, the Equal Rights Amendment passed the U.S. Senate, and there was a “burglary” at the Watergate Hotel in D. C. At Pitt, the Chemistry Department hosted a symposium on the *Physical Chemistry of Aqueous Systems* to honor the 70th birthday of Professor Henry Frank.

Richard Bertozzi (PhD '72; Advisor: Coetzee) was the V.P. of R&D Toiletries Tech Lab at Gillette before his retirement. He is widowed and re-married in 2010 to a wonderful Argentine lady. He had a U. S. Patent Awarded in 11-02-10. (richbertozzi@msn.com)

Richard J. Colton (BS '72, PhD '76; Advisor: Rabalais) is the Superintendent, Chemistry Division at the Naval Research Laboratory. He was the Director of NRL's Institute for Nanoscience before becoming head of the Chemistry Division in 2007. Recent awards include the 2011 Navy Superior civilian Service Award and Pitt's Chemistry Department's Distinguished Alumni Award. (adcolton@cox.net)

Edward H. Conrad (BS '72, MS '80; Advisors: Douglas and Frohlinger). After obtaining a MS Degree in Hygiene in 1980 from the University of Pittsburgh, Graduate School of Public Health, Edward began his career in industrial hygiene at Gulf Oil Corporation in Harmarville, PA. Subsequent positions in the industrial hygiene field were held with Marathon Oil Company, Koppers Company, Westinghouse Electric Corporation, and finally Bayer Corporation - all in the Pittsburgh area. Ed served as the president of the Pittsburgh section of the American Industrial Hygiene Association in the 1990's. He retired from Bayer Corporation in 2009.

Robert Louis Cross (BS '72): (B05CR@comcast.net)

Maryanne McClosky Debies (BS '72; Advisor: Pan) has retired from Xerox Corp. where she was an environment, health and safety manager for research. She moved back to the Pittsburgh area early in 2012. She has been married to Thomas Paul Debies (Chem '71 BS and PhD '75) for 37 years. They have two adult children and 2 grandchildren. (maryannedebies@yahoo.com)

Thomas W. Hill (MS '72; Advisor: Wallace) is the Chairman at Microseeps, Inc. He is having fun in the environmental lab-business with niche analyses in support of natural attenuation (NA) and isotope analyses (CSIA). He has been married for 32 years and has two children: Matt who is working for the University of Chicago, and Manny who is a senior at University of Michigan. (thill@microseeps.com)

R. Douglas Hutchens (PhD '72; Advisor: Wallace) is the Director of Academic Research at Universal Technology Corp. Currently he manages a Congressionally mandated 9 year research program to enhance minority participation. He is married with two sons and five grandchildren. (rdhutchens@earthlink.net)

Dale E. Johnston M.D. (BS '72, MS '75; Advisor: Arnett) is a Diagnostic Radiologist at Radiology Associates, P.A. Little Rock, AR. He did his Diagnostic Radiology residency at Washington University (St. Louis 1979-83), and he is married to former Janice Davis BS '74. They have three children; their oldest daughter is a technical writer at Bechtel – Bettis in West Mifflin, PA. (DEJ82552@aol.com)

George W. Luther III (PhD '72; Advisor: Carter) is the Harrington Professor of Marine Study at the University of Delaware, where he performs research in the area of marine chemistry. He has published over 200 research articles and won numerous honors for his research. George and BJ are enjoying life at Rehoboth Beach, DE, when he is not traveling to perform research on deep sea hydrothermal vents and the Black Sea.

Michael G. Sheppo (MS '72 Forensic Chemistry) has worked in forensic sciences since 1972, and he is currently the Director of the “Office of Investigative and Forensic Sciences” at the National Institute of Justice. Michael is active in several professional societies, and serves as a speaker on numerous forensic science topics. Michael resides in Silver Springs, MD and works in D.C.

Albert J. (Bert) Smith (BS '72; Advisor: Kaufman) went on to receive his MBA in 1974. He worked for 34 years at Alcoa, first as a systems analyst and later as a management accountant. He now works at NuGo Nutrition. He and his wife Linda have been married since 1987 and have two children, Emily and Nathan. His favorite chemistry professors were Dr. Alfred Moyé and Dr. Foil Miller.

Christine Starcevic Tomsey (MS '72; Advisor: Epstein) was the Lab Director & DNA Technical Leader at the Pennsylvania State Police-DNA Laboratory before retiring after 35 years. She established and directed the DNA laboratory within the Bureau of Forensic Services of the State Police. (carts7@comcast.net)

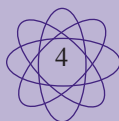
Michael Swerdloff (PhD '72; Advisor: Cohen) is the manager of Staffing Services at Novartis Pharmaceuticals Corp. After a career in bioorganic research, he switched to recruiting scientists for then Sandoz Pharmaceuticals Corp. After Sandoz merged with CIBA-GEIGY to form Novartis Pharmaceuticals Corporation, he switched into recruiting clinical and medical personnel, which he now does almost exclusively. (mike.swerdloff@novartis.com and tennisball2000@hotmail.com)

Daniel W. Trainor (PhD '72 Physical Chemistry; Advisor: Kaufman) retired from his position as Senior Director of Laser Technology at Textron Defense Systems. (Wilmington, MT) in the winter of 2010. Over the years his research work led to a number of new lasers and laser concepts, including the basic laser research (excimer lasers) that is used in eye corrective surgery.

James J. Valentini (BS '72; Advisors: Carter, Siska, and Danishefsky) is a Professor of Chemistry and Dean of Columbia College and Vice President for undergraduate education at Columbia University. Web address: www.college.columbia.edu/about. (jjv1@columbia.edu)

Robert A. Volkmann (PhD '72 Synthetic Chemistry; Advisor: Danishefsky) worked at Pfizer from 1974 to 2009 and is employed now at CSO Systemolic Inc. Bob has 48 research publications and over 35 patents from his work in organic chemistry and drug discovery.

James E. Williams, Jr. (MS '72) was the Director of Adv. Tech. at Seagate before his retirement in 2007. Since that time, James has served as a consultant for the Data Storage Systems Center at CMU. James holds four patents and has authored several technical papers and book chapters. He has received several awards for his accomplishments.



Alumni Updates

Harold Bryant (PhD '91; Advisor: Weber): Dr. Bryant is currently a VP in Research and Innovation at L'Oreal in NJ. He leads a team of 60 people in three groups, including analytical chemistry, microbiology, and demi-grand. The demi-grand is a pilot plant responsible for the scale-up of bench processes to 300 kg. Together, the three groups are responsible for supporting development and innovation processes by assuring the robustness of preservative systems in proposed formulations, by troubleshooting processes, by addressing finished product issues and raw material concerns, and by managing the control and supply of all raw materials supplied to the bench chemist on-site.

Jolie DeForrest (PhD '09; Advisor: Brummond): Dr. DeForrest is studying for the New Jersey bar and getting ready to move to D.C. in August, where she has a job with an intellectual property law firm. In other news, she recently published a paper regarding the obviousness of structurally-related compounds with respect to patentability. In particular, her paper focused on the design and development of Singular and Gemzar.

Dominic M. Desiderio (BS '61) Phd '65 from MIT taught 11 years at Baylor College of Medicine. Since 1978, he has been a Professor in the Department of Neurology, Professor of Molecular Sciences in the Department of Molecular Sciences, and Director of the Charles B. Stout Neuroscience Mass Spectrometry Laboratory at the University of Tennessee Health Science Center. He is a co-editor of the Wiley journal *Mass Spectrometry Reviews*, a co-editor of the Wiley Book- Series on Mass Spectrometry, and an Associate Editor of the EPMA journal.

Claudia B. Cohen Jaffe (PhD '93; Advisor: Weber): Dr. Jaffe has founded a solid state lighting company, Lumencor, Inc. in Beaverton Oregon. They manufacture illumination subsystems for a broad array of bioanalytical instruments including fluorescent microscopes, high content screening, microarray and microfluidic readers, slide and chip scanners, digital pathology, endoscopes, and a host of other applications that require high performance excitation light. She manages the organizations' business development, sales, and marketing teams and also is a key contributor to the IP portfolio of Lumencor.

Amanda C. Kasper (BS '05): PhD '10 from Duke University in Organic Chemistry. Dr. Kasper is the Duke University Lab Manager for all Organic Chemistry Labs.

Kristi O'Neal Kauffman (PhD '09; Advisor: Weber): Dr. Kauffman is currently working in the Analytical Shared Services Department at PPG Industries. She is the team leader of the Methods and Materials Characterization group, which combines unique sample preparation techniques with spectroscopic analysis to provide fundamental understanding in support of new product development. The group focuses on new method development, structural analysis of polymers, and reverse engineering of coatings products.

Shu Li (PhD '99): Dr. Li is working with Novartis (Cambridge, MA) in support of Novartis' drug discovery efforts. His work in analysis (assay, metabolomics) supports target identification and validations.

John Orr (BS '84): John is working at Eisai Pharmaceuticals, with another Pitt alumnus, Dr. Hui Fang. They are members of the Analytical Chemistry group and have responsibility in the design of analytical techniques used to ensure the quality of the drug substances. They also design analytical methods for monitoring the chemical transformations utilized in the synthesis of drug substances. Recently, they gained approval for an oncology agent, Halaven, for the treatment of breast cancer.

Joshua Osbourn (PhD '12; Advisor: Brummond): Joshua has accepted a position as an assistant professor on the teaching faculty at WVU.

Eskil Sahlin (Postdoc '01; Advisor: Weber): Dr. Sahlin works at SP Technical Research Institute of Sweden where he performs different chemical analyses (mainly inorganic). He also develops new analytical methods and modifies existing methods when it is needed. He is also involved in the teaching of chemical metrology and advising in chemical analysis issues.

Yuanhua Shao (Postdoc '96; Advisor: Weber): Dr. Shao returned to China as a Research Professor at Changchun Institute of Applied Chemistry for 4-years. He then moved to Peking University as the Changjiang Professor of Chemistry in 2002. He currently focuses on research of electrochemistry at soft interfaces.

Guoyue Shi (Postdoc '05; Advisors: Weber, Michael): Dr. Shi is Professor and Chair of the Department of Chemistry at East China Normal University, Shanghai, China.

Carol D. (Guerrero) Shreiner (BS '99): Carol is an Assistant Professor of Chemistry at Hiram College.

J. Matthew Simon (PhD '69): Dr. Simon is retired President and Distinguished Service Professor at Point Park University. He was appointed in 2005 to be a member of the Financial Oversight Authority (ICA) for the City of Pittsburgh. ICA is mandated by the Commonwealth to assist the city in reaching sustainable financial stability.

Wanlin Xia (PhD '99; Advisor: Weber): Dr. Xia is currently working in Asymchem, a CMO headquartered in Morrisville, NC with manufacturing capacity located in China. His primary responsibilities are analytical support for advanced intermediates, drug substances, and drug products.

Xiaomi Xu (PhD '11; Advisor: Weber): Xiaomi is a procurement engineer at Agilent. Her main role is to ensure the quality of Agilent products procured from suppliers.

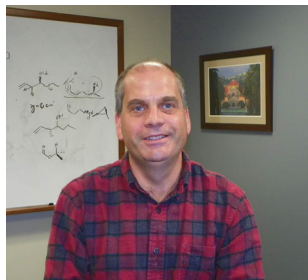
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the Department of Chemistry
Facebook page*

[www.facebook.com/
pittchemdepartment](http://www.facebook.com/pittchemdepartment)

*Stay connected with
Department news and events.*



Faculty Highlights: Paul Floreancig

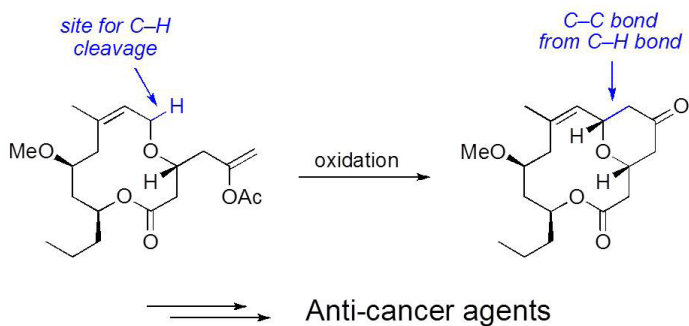


Chemistry Professor Paul Floreancig and his group are engaged in the multifaceted area of organic synthesis. Their work is directed toward devising fundamentally new chemical transformations, applying these transformations to the synthesis of structurally complex biologically active materials, and engaging in collaborative efforts to enhance the potency of naturally-derived anti-cancer agents. Professor Floreancig is also actively involved with the University Honors College and has taught the Honors Organic Chemistry sequence for the past several years.

Oxidative Carbon–Hydrogen Bond Functionalization

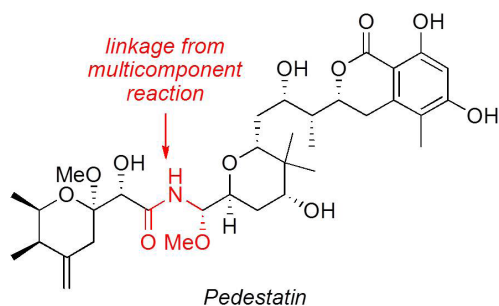
Carbon–hydrogen bonds are ubiquitous in organic molecules. The conversion of carbon–hydrogen bonds to carbon–carbon bonds provides an attractive and effective approach to increasing molecular complexity. This strategy is complicated by selectivity issues – i.e. how can a single carbon–hydrogen bond be targeted for functionalization in the presence of several similar bonds? The

Floreancig group has developed several models for predicting the reactivity of carbon–hydrogen bonds toward oxidative cleavage, leading to a useful and predictable way to form versatile carbocation intermediates. This strategy has been used to prepare the anti-cancer agent neopeltolide and the potent analog 8-hydroxy neopeltolide.



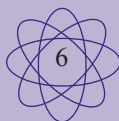
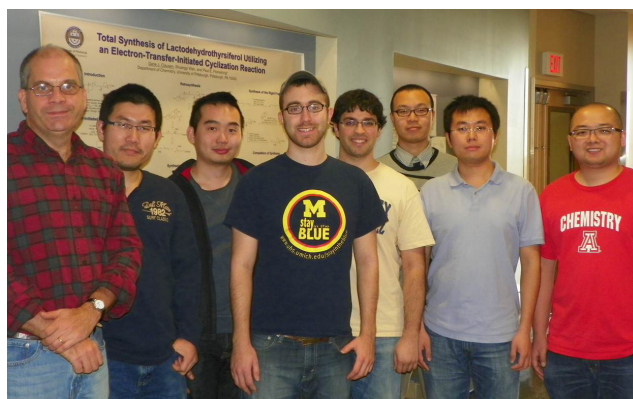
Multicomponent reactions

Multicomponent reactions allow for complex structures to be built quickly and also create the possibility for rapid structural diversification that is useful for biological activity studies. They have exploited nitriles as useful substrates in multicomponent reactions that lead to amide products. This has allowed them to prepare a number of structurally unique small molecules for biological activity screening studies. They have also used this protocol to study the structural requirements for the anti-cancer activity of the natural products pederin and psymberin. This study resulted in the preparation of pedestatin, which is an extremely potent agent for killing cancer cells.



Honors Organic Chemistry

The purpose of the Honors Organic Chemistry sequence is to provide students with an opportunity to pursue important concepts at a deep level, to learn about modern aspects of organic chemistry, and to explore the relationships between fundamental chemical principles and observed phenomena in biology, medicine, energy, and nanoscience. The relatively small class size allows students to direct the flow of discussions in an interactive environment.



Faculty Nuggets

Sanford Asher won the Charles E. Kaufman Foundation 2011 Award for his fundamental research that has advanced the field of knowledge and benefited humankind through technologies of economic value and significance for improving human welfare, health, and security. Professor Asher was presented with this \$50,000 award in December of 2011.

Kay Brummond's recent paper, *A Thermal Dehydrogenative Diels-Alder Reaction of Styrenes for the Concise Synthesis of Functionalized Naphthalenes* (Org. Lett. 2012, 14, 4430-4433) was highlighted in a recent issue of SYNFACTS (issue 11/12) for its important insights.

Lillian Chong was selected as a recipient of a 2012 Carnegie Science Emerging Female Scientist Award. The Emerging Female Scientist Award recognizes a female leader whose cutting-edge work inspires change in math, science, or technology.

Sean Garrett-Roe received the 2012 Spectroscopy Society of Pittsburgh Starter Grant Award to develop new spectroscopic methods that will investigate how next-generation solar cells will work.

Seth Horne was granted a National Science Foundation CAREER award for his proposal entitled "*Supramolecular Light-Harvesting Materials from Self-Assembly of Bio-Inspired Macromolecules*." The NSF Faculty Early Career Development (CAREER) Program offers the Foundation's most prestigious awards in support of junior faculty who exemplify the role of teacher-scholars through outstanding research, excellent education, and the integration of education and research.

Geoff Hutchison was selected to receive a Research Corporation for Science Advancement 2012 Cottrell Scholar Award based on his proposal entitled "*Molecular Piezoelectrics: Building Responsive Electromechanical Materials from the Bottom Up*."

Kenneth Jordan was elected as the Vice-Chair of the Division of Computational Physics of the American Physical Society.

Xinyu Liu was awarded a career development award from Melanoma & Skin Cancer SPORE at UPCI, for his proposed research on the structural and functional study of glycosylation on antigenic proteoglycan related to melanoma pathogenesis.

Jill Millstone was chosen to be a participant in the CSC New Faculty Workshop that took place in Washington, DC. in the ACS National Offices on August 9-10, 2012.

Nathaniel Rosi was selected as a Kavli Fellow for 2012 and participated in the German-American Kavli Frontiers of Science symposium in Potsdam, Germany. Kavli Fellows are selected by a committee of National Academy members from young researchers who have made recognized contributions to science.

Sunil Saxena has won the 2012 Tina and David Bellet Teaching Excellence Award which recognizes outstanding and innovative undergraduate teaching in the Dietrich School of Arts and Sciences.

David Waldeck was a speaker at TedxPittsburgh (<http://www.tedx-pittsburgh.com/presenters/WaldekDavid.asp>). His talk, *Solar Paint*, described the use of chemistry and nanoparticles to create flexible composite materials that act as a photovoltaic material to generate electricity from sunlight.

Michelle M. Ward was named Editor with the National Council of Iota Sigma Pi - National Honor Society for Women in Chemistry.

Stephen Weber received the 2012 Provost's Award for Excellence in Mentoring. The Award is given annually and recognizes up to four members of the graduate faculty for outstanding mentoring of graduate students seeking a research doctorate degree.

Peter Wipf is the 2012 winner of the ACS Pittsburgh Section Award. The Pittsburgh Award was established in 1932 to recognize outstanding leadership and distinguished service to the field of chemistry in the local and larger professional community. The Award consists of a plaque and will be presented at a special ceremony on Tuesday December 11, 2012 at the DoubleTree by Hilton Hotel in Greentree.



Graduate Highlights: Jessica Sarver



Jessica Sarver received her Ph.D. in Chemistry this past spring. Her research in biophysical chemistry was performed under the guidance of Sunil Saxena and focused on resolving the structure and function of protein systems using electron spin resonance. During her time at Pitt, Jessica received both the Safford Teaching Fellowship and the Safford Teaching Award. She also received travel awards and gave oral presentations of her work at the Rocky Mountain EPR Conference in Snowmass, CO in 2009 and 2011 as well as at the national APS meeting in Pittsburgh in 2009. Jessica also gave a departmental seminar at Penn State Behrend, her alma mater, in 2008.

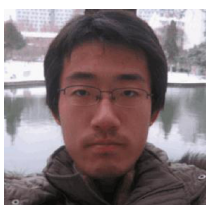
Jessica's thesis is entitled "Probing the Structure and Dynamics of a Protein-DNA Complex Using Electron Spin Resonance". Her experimental studies of EcoRI investigated how the structure and dynamics of the DNA-binding protein changed when bound to different sequences of DNA. She used correlated distance constraints and MD simulations to reveal, the preferred conformations of the nitroxide spin label on sites in an α -helix and a β -strand and to gain information on the backbone motion at spin-labeled sites in the EcoRI-DNA complex.

While at the Pitt, Jessica took part in numerous teaching and service opportunities. Jessica was a teaching assistant for the general chemistry course as well as for the analytical chemistry laboratory course. Jessica was also the teaching assistant mentor for general chemistry. In addition, she was a chemistry tutor for undergraduate students, taught college in high school labs, participated in the TA training for general chemistry, and volunteered for the Chemistry Olympics for several years. Jessica served as the PLU president (2008-2010) and was a member of the Graduate Student Organization (2008-2010) and the Chemistry Department Budget and Finance Committee (2008-2010).

This summer Jessica accepted a postdoctoral position in David Cafiso's lab at the University of Virginia where she continues to investigate biological systems using magnetic resonance techniques.



Bayer Materials Science Fellowship



The Bayer Corporation's long-standing association with the Department of Chemistry has provided significant benefits, including the Bayer Lecture Series and fellowship support of graduate students in the program. Since 2009, the Bayer Foundation grant program has provided fellowship support to seven qualified graduate students whose research interests are focused on material science. Current recipients of these fellowships include Hyo Jeong Kim (Prof. Haitao Liu's group) whose research interest is polymers/macromolecular chemistry and Yong Zhao (Prof. Alexander Star's group) whose focus is on nanomaterials and processes.



Since 1979, the Bayer Lectures have provided the Department with the opportunity to host noted scientific experts whose exceptional presentations have highlighted our colloquium series. This year's speaker, Prof. Daniel Nocera of MIT, drew standing room only crowds to the Ashe Lecture Hall for his talks on "The Global Energy Challenge" and "The Artificial Leaf".

The Department of Chemistry is proud to maintain our association with Bayer in the 21st century.

Graduate Awards

School of Arts & Sciences Andrew Mellon Predoctoral Fellowship

Kara George-Rosenker
Matthew Zwier

Goldblatt Fellowship

Vamsee Voora

Bayer Material Science Fellowship

Yong Zhao
Hyo-Jeong Kim

BASF Graduate Excellence Award

Liming Cao
Sean Gardner

Basu Endowment Award

Laura Kocsis

Graduate Excellence Fellowship

Liqing Gu
Tao Li
Brandon Parks
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Youwei Xie



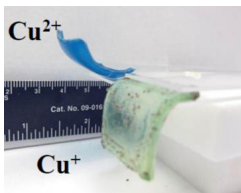
Undergraduate In The Spotlight:

On Sunday, April 29, 2012, the Department of Chemistry celebrated the achievements of our graduating seniors. Rachel Harris was a member of this wonderful group of students. Rachel graduated this past April with an ACS Certified chemistry degree and University and Departmental Honors. During her undergraduate career, Rachel received many awards in recognition of her contributions to our department: both academic and service-related. Among these are the Dunkelberger Award, given for outstanding outreach commitment, and the Theodore Prize, given for outstanding overall performance by a graduating senior. Rachel carried out undergraduate research under the direction of Professor Tara Meyer in the area of stimulus-responsive materials. The photo shows an example of a hydrogel she developed that changes its stiffness with redox state of its copper metal ion. Rachel received the ACS Inorganic Award in recognition of this work. She was also very involved in our undergraduate teaching program, where she led recitations for students in Organic Chemistry lecture classes, and mentored students in the Honors Organic Laboratory course. Rachel also showed her dedication to our department by serving as Co-President (along with Joshua Glass) of our nationally recognized American Chemical Society-Student Affiliates group. Rachel began graduate studies in Materials Chemistry at Northwestern University this fall.



We wish Rachel and all of our new alumni great success in their future endeavors, and we hope that they will carry on our department's commitment to the community as they pursue their life goals.

The photo shows how a hydrogel's mechanical strength changes with the metal ion's oxidation state. The Cu^{2+} hydrogel is a tough but flexible material whereas the Cu^+ hydrogel is soft and bends in response to gravity.



ACS-Student Affiliate

The ACS-SA is a vital part of the University of Pittsburgh's undergraduate chemistry community. Throughout the year it hosts a variety of speakers, holds social events, and coordinates community outreach efforts so that we can share our passion for chemistry and science with others. Although largely chemistry majors, the organization's reputation for leadership and outreach activities attracts members from a variety of majors such as engineering, neuroscience, psychology, and biology.

The ACS-SA has a number of goals for the upcoming year. This year the ACS-SA is moving to strengthen ties with the honorary chemical society for graduate students, Phi Lambda Upsilon. The objectives and goals of the PLU and the ACS-SA are well aligned. Through collaboration we hope to increase the participation in volunteer efforts and strengthen the connection between undergraduate students and graduate students. This year the ACS-SA is starting outreach efforts at St. Benedict's Catholic School and St. Rosalia's Catholic School to provide hands on science experience to elementary and middle school students. ACS-SA will continue its efforts to promote green chemistry by seeking out speakers from companies that promote sustainable and/or environmentally benign activities and by printing weekly green chemistry articles in our newsletter. We will also continue to participate in the many available outreach programs, such as Saturday Science, National Chemistry Week, the Chemistry Olympics, chemistry tutoring, and teaching honors high school lab classes.

2012 Undergraduate Awards

The American Institute of Chemists Award
Terry L. Paske

The Mary Louise Theodore Prize
Valerie J. Alstadt
Kiersten A. Bendzłowicz
Joshua M. Glass
Rachel D. Harris
Nicholas A. Naro
Keith A. Werling

The Merck Award
David W. R. Wang
Samuel Zolin

The SACP College Award
Mark T. Kozłowski

The Silverman Prize
Catherine M. Madden

The Phillips Medal
Matthew Y. Zhu

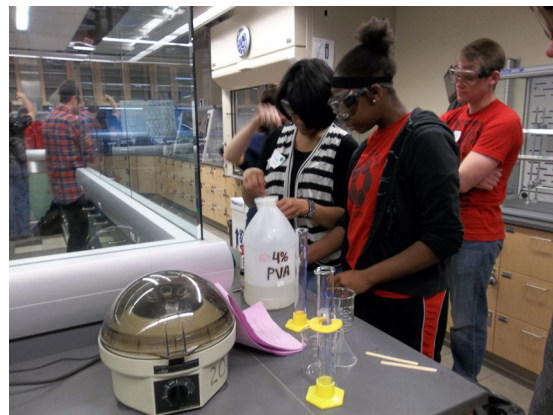
Outreach:

Chemistry Department Breaks the Mold of Outreach Programs

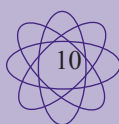
It is early on a Saturday morning, yet there is a flurry of activity and excited voices coming from a lab on the second floor of the Chevron Science Center. Some high school students are busy combining two clear solutions to make a polymer in one corner of the lab, while others are huddled around a table mixing iron and luminol to create a substance that gives off an eerie glow.

Under the guidance of undergraduate chemistry students, the Saturday Science Academy provides local high school students from groups typically underrepresented in science with a fun, hands-on laboratory experience, and it exposes them to some basic principles of synthetic and analytical chemistry. Some of the many experiments include making crystal gardens, measuring the pH levels of favorite soft drinks, and synthesizing slime.

The Saturday Science Academy is one of many outreach programs available to area elementary, middle, and high school students offered through the Department of Chemistry's American Chemical Society-Student Affiliates (ACS-SA) group. ACS-SA, open to all majors and disciplines, is a vibrant and active undergraduate organization. Students involved in ACS-SA are dedicated to fostering a greater knowledge of the field of chemistry as well as igniting curiosity and passion for the sciences.



“Outreach is a vital part of a student’s total education at Pitt,” says George Bandik, Director of Undergraduate Studies for the Chemistry Department. “It is our responsibility as educators to provide the necessary tools to help students become good citizens and great people.” ACS-SA meets weekly and provides a wonderful opportunity for networking, not only with students from other disciplines but also with faculty and industry leaders. A lecture series in the fall is devoted to post graduation opportunities and invites career counselors, graduate and professional school advisors, and industry representatives to speak to the students. ACS-SA members also volunteer as tutors and assist undergraduate students in general or organic chemistry. The organization is open to any student interested in the sciences, from anthropology to zoology.





Bandik, who also is the faculty advisor for ACS-SA, is passionate about student involvement in academically based organizations. “These outreach programs provide a great learning experience and allow students to give back to the community,” says Bandik. “In fact, many of our former students, who include Rhodes and Churchill scholars, made time in their schedules to be involved in community outreach programs. Whether students are supervising experiments at area schools or reaching out to their peers in the

classroom, it is all about service to others.”

Service, education, and research are the foundation of the University of Pittsburgh and the heart of the Department of Chemistry’s undergraduate program.

The Department of Chemistry offers teaching and research opportunities for undergraduate students as well. The Undergraduates Teaching Undergraduates program is a peer-teaching activity for trained undergraduates who want to help other students by acting as recitation or lab instructors in general chemistry classes or lab instructors in organic chemistry sections. Many undergraduate research opportunities are available inside and outside the Department and over three-fourths of our graduating seniors perform research during their time in the program. Because chemistry is a lab science, it is essential for students to participate in lab research, which ties together course work and hands-on experiences.

This article originally appeared in The Pitt Pride (Volume 6, Issue 1). It has been edited and adapted with permission.

Department Milestones: New Faculty – Daniel S. Lambrecht – Assistant Professor



Professor Daniel Lambrecht comes to us from the University of California at Berkeley, where he completed his postdoctoral work on electronic structure theory and *ab initio* molecular dynamics of solvation clusters in the group of Martin Head-Gordon. He received his undergraduate degree in Chemistry from the University of Düsseldorf, Germany, in 2003. In the same year, he moved to the University of Tübingen, Germany, to carry out his Ph.D. research on the development of efficient electronic structure methods for accurate

calculations on molecules with 1,000 and more atoms, under the direction of Christian Ochsenfeld (now University of Munich). In 2001, Dr. Lambrecht spent one year at the University of North Carolina at Chapel Hill as an exchange student.

Daniel’s current research focuses on the computational description of chemical binding and reactions in the condensed phase, with the goal of developing techniques for the rational design of catalysts and materials for use in alternative energy systems.

Dr. Lambrecht has 18 publications including a book chapter in *Reviews in Computational Chemistry*. This fall Professor Lambrecht is teaching Chem 2430, Quantum Mechanics and Kinetics, a course on the application of quantum mechanics in chemistry.

Staff Retirements –

This past summer six long time staff members chose to take advantage of a voluntary early retirement program. We wish all of them well in their retirement from Pitt.

Lynne Clemente (October 1998) Lynne worked with Prof. Dennis P. Curran and his research group for all of her fourteen years in the Department. During that time, she assisted Prof. Curran in all aspects of his work (research, teaching, service), and she was the ‘go-to’ person for group members to solve all kinds of problems. She was widely appreciated for knowledge of procedures, her efficiency, and her friendliness. Lynne plans to relax and enjoy her family, especially her newly born first granddaughter.



Bill Grisom (December 1974) Bill was hired as Research Stockroom Store Clerk and 38 years later retired as Research Stockroom Manager. Bill managed the stockroom through many changes of the purchasing process and procedures. Bill was always available as a friendly resource and willing to offer a wry sense of humor.



Fran Nagy (October 1992) Fran was part of the Department of Chemistry for 20 years. Originally hired as part of the Department’s secretarial staff, she became the Graduate Administrator in 1999 and was responsible for over 200 graduate students. In 2008 Fran received the Chancellor’s Award for Staff Excellence in Service to the University, an award that recognizes staff who consistently exceed standards and expectations set for their position. The graduate students always looked forward to receiving their ‘star’ from Fran when they passed their dissertation defense and graduated with a PhD from the Department of Chemistry. Fran’s retirement plans are to relax with her husband and spend more time visiting her daughters.



Larry Suckfield (September 1986) Larry was hired as a store clerk for the Research Stockroom of the Chemistry Department. For 26 years Larry greeted faculty and graduate students, filled their orders, sorted and delivered the mail, received and delivered packages, and kept the shelves stocked with beakers, reagents, office supplies, and more. Larry plans to take on a part time job in the near future.



Roy Watters (June 1980) Roy was first hired in the Chemistry Department Machine Shop as a Scientific Instrument Maker. He remained in the Department for 32 years, and he retired as a Precision Production III machinist. He plans to reside in southwestern PA and in Florida. Roy is a nationally known locksmith and will continue to operate his locksmith business. He also plans to do some fishing, which should provide much new material for his portfolio of stories.



Toni Weber (October 1985) Toni began working at the University of Pittsburgh in March 1981 in the Payroll Department as an Accounting Clerk, transferred to the Library and Information Sciences Department, and then to the General Accounting Department. In November 1985, she was recruited by Dick Howe (who was the Chemistry Department’s Assistant Chair at that time) to begin working in the Chemistry Department in a payroll/personnel position. She remained in the Chemistry Department for the next 27 years. Toni and her husband have just returned from a ‘retirement celebration’ cruise. She is planning to spend more time with her husband and her family, and to relax with a paint brush and canvas.



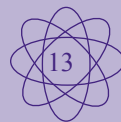
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Renovation Updates

Updates to our facilities continue and are providing the Department with modern laboratory space that enriches our instruction and enhances our research. In fact, the Chemistry Annex was selected for a 2012 “Honor Award” by the SCUP/AIA-CAE Excellence in Architecture program. (<http://www.scup.org/page/awards/2012/recipient/award15>) Also, the American Institute of Architects (AIA) Pittsburgh bestowed “Honor Awards” on the Chemistry Annex in the architecture category and on the Undergraduate Chemistry Labs in the interior architecture category during their *Design Pittsburgh* event, which is a celebration of architecture and design. (<http://alaphg.org/feature-articles/design-pittsburgh-2012/>)

During the past year, two third-floor General Chemistry teaching labs in the Chevron Science Center were remodeled to accommodate both General Chemistry and Organic Chemistry Laboratory classes. The layout of these dual-purpose labs provides an inner core for recitation, report preparation, and “non-chemical” activities that are separate from the experimental area which is composed of bench space around the periphery of the rooms. The fume hoods in these labs allow them to be used safely for both General Chemistry and Organic Chemistry experiments and studies.



Third Floor Teaching Labs

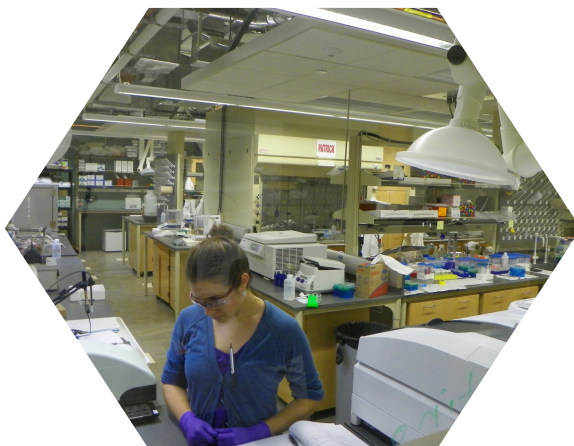
To provide support for all Arts & Sciences departments, the machine shops in Chemistry and Physics and Astronomy were recently merged and are now housed in NPL (the former Nuclear Physics Laboratory) building. Space that was formerly occupied by the machine shop was completely gutted and converted into the new Chemistry Instrumentation Center (CIC). This space provides a bright, spacious, central location for housing the Department's NMR, X-Ray, and Mass Spectrometry facilities. Construction of this space was completed in early November. A phased relocation of equipment is underway and expected to be completed in January 2013.



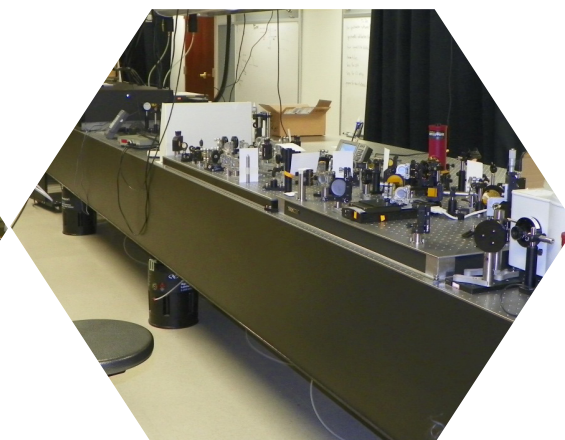
Chemistry Instrumentation Center

www.chem.pitt.edu

This past winter labs on 10th floor were remodeled and are being used by Prof. Jill Millstone and her research group who work in nanomaterials synthesis; and labs on the second floor of Eberly Hall (formerly the Chemistry Library location) were converted into an ultrafast laser spectroscopy lab for Prof. Sean Garrett-Roe and his research group.



Prof. Millstone Lab

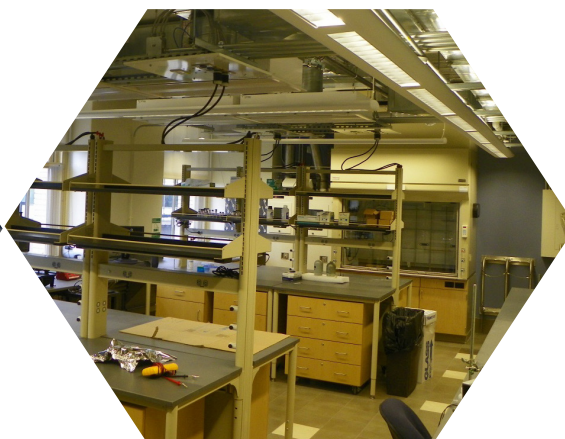


Prof. Garrett-Roe Lab

The purchase of w-band Electron Paramagnetic Resonance (EPR) spectrometer, funded by an award to Prof. Sunil Saxena, resulted in an upgrade to the existing EPR lab in Chevron. Renovation of the lab space has been completed and new spectrometer is scheduled for installation in January of 2013. Finally, to provide additional research space for the expansion of Prof. Alex Star's program, a lab in Eberly has been remodeled and is equipped for measurements of nanomaterials and the evaluation of sensors based on nanomaterials.



New EPR Facility



Nanomaterial Sensor Lab



University of Pittsburgh

*Kenneth P. Dietrich School of Arts and Sciences
Department of Chemistry
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We look forward to hearing from you!

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