Department of Chemistry Newsletter

Greetings from the Chair

s each new academic year unfolds, it seems as though the political and financial landscape presents us with new challenges and new opportunities. Yet our core principles remain the same; namely, a focus on the education of our students, the mission of the University of Pittsburgh, and the advancement of chemistry as a discipline—a commitment to excellence.

The University continues to invest in the Department's infrastructure. We are proud of the newly renovated areas of the Chevron/ Ashe/Eberly complex that are providing stateof-the-art graduate research environments, modern undergraduate laboratories designed for function and safety, an up-to-date computer classroom, and inviting and comfortable spaces in which to study or to interact. Noteworthy accomplishments this year are the newly renovated second floor general chemistry labs, the fifth floor research space, and the Annex with its two research floors (see pgs. 14, 15). We are looking forward to further improvements of the Department's facilities and technical resources that are currently in the planning stages.

The Department's quality is reflected in that of its faculty and staff (see pgs 6, 7, 10, and 11). We extend our best wishes to Prof. David Pratt on his retirement, as we welcome our newest tenure stream faculty members, Jill Millstone and Sean Garrett-Roe. Dr. Millstone's research focuses on the study of nanostructure surface architectures, with the goal of developing highly tailored materials for use in medical devices and alternative energy systems. Dr. Garrett-Roe's emphasis is the development of multidimensional (2D and 3D) IR spectroscopy to study ion uptake and selectivity in ion channels, ion sensors, and ionophores. These changes increase the department's number of tenure stream faculty to 31, as we continue to expand and enhance the scope of our graduate research. We also welcome Dr. Bhaskar Godugu as the director of our Mass Spectrometry support facility, and Dr. Carol Fortney and Dr. Susan Maleckar as full-time lecturers, to support our undergraduate teaching mission.

Most important to a Department's quality is the excellence of its students and their accomplishments during their careers. Our graduate and undergraduate programs remain vibrant. With 41 PhD candidates matriculating this fall, the graduate program remains robust with over 200 graduate students and 37 postdoctoral associates involved in research. The Department conferred 27 PhD and eight MSc degrees during the past year. Our highly ranked undergraduate program remains a source of pride and has shown renewed growth in recent years, with 263 chemistry majors in residence and 71 BSc degrees conferred in the past year! Beyond growth in size, the quality of the Department's students and alumni continues to be evident in their individual accomplishments (vide infra).

The Department has launched and supported several new initiatives to encourage and support the involvement of underrepresented minorities (URM) and women in chemistry from the undergraduate to the graduate level. The Department hosts a local chapter of NOBCChE (National Organization of Black Chemists and Chemical Engineers) with student members from Pitt, CMU, and Duquesne universities. Dr. Muscatello and others have created a Pittsburgh section of the American Chemical Society Women Chemists Committee (ACS-WCC) (see pg. 12).

Commitment, engagement, scientific excellence—these are hallmarks and traditions of the Department that will continue for years to come. We thank alumni and friends for the generous support the Department receives and extend our best wishes to you.

David H. Walder



Issue 8 Fall 2011

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CALL FOR NOMINATIONS

The Department is soliciting nominations for the 2012 Department of Chemistry 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 www.chem.pitt.edu for more information

Nominations should be posted by

January 4, 2012

University of Pittsburgh Department of Chemistry Assistant Chair Pittsburgh, PA 15260

Outstanding Alumnus: Nadrian C. Seeman

The structure and self-assembly characteristics of DNA-based nanomaterials and nanoscale objects is the theme of Prof. Nadrian C. (Ned) Seeman's research program. Ned Seeman received his BS in biochemistry from the University of Chicago in 1966 and his PhD in crystallography/biochemistry from the University of Pittsburgh in 1970 where he worked with Professor George Jeffrey; his thesis was entitled, "The Use of Patterson Superposition Techniques in the Interpretation of the X-Ray Diffraction Data of Crystalline Beta-(Pyrazolyl-3)-L-Alanine and 1,6: 2,3-Di-Anhydro Beta-D-Gulopyranose and the Application of Patterson Rotation Functions to the Comparison of Structures Composed of Similar Units." Ned is currently the Margaret and Herman Sokol Professor of Chemistry at New York University and the progenitor of structural DNA nanotechnology.

After obtaining his PhD, Ned took postdoctoral positions at Columbia and then at MIT before taking a faculty position at SUNY, Albany. While at Albany he laid the foundation for the structural DNA nanotechnology field by focusing on the self-assembly of DNA to form well-defined and predictable species, particularly crystals. Following his move to NYU, his group's first construct of a closed polyhedral object from DNA (a cube) was reported in 1991 "Synthesis from DNA of a molecule with the connectivity of a cube", *Nature* 350 (1991) 631. Since that time the idea of using DNA as a 'tinkertoy' to design self-assembling objects, lattices, and nanomechanical devices has blossomed. While applications of these materials are yet to be identi-

fied, they are providing an intellectual training ground for understanding how to design and self-assemble three-dimensional supramolecular objects with structural fidelity and function. Ned's research has continued to focus on the self-assembly of DNA molecules into three-dimensional crystalline arrays and their associated biophysics. His construction of nanoscale materials and mechanical devices, and the work by others he has inspired, has led to extensive study of the structure, dynamics, and thermodynamics of DNA-based materials. See Ned's Web site to learn more about his ground-breaking research (http://seemanlab4.chem.nyu.edu/).



Ned has received numerous honors and awards, most recently the Kavli Prize in Nanoscience (2010), shared with Donald Eigler of IBM's Almaden Research Center, for the development of "methods to control matter on the nanoscale."

While at Pittsburgh, Ned Seeman was a student with Professor George A. Jeffrey. George Jeffrey came to the Department of Chemistry as a faculty member and established a crys-

tallography laboratory in 1953. From its inception, this laboratory grew, becoming its own department in 1969. The first of its kind in the United States, the Department of Crystallography was renowned for the solution of many complex crystal structures, particularly those of carbohydrates, cholesterols, and clathrate compounds. In addition to Ned Seeman, the crystallography program trained a cadre of impressive research scientists (76 PhD students and 7 MSc students); two of whom, Helen Berman (PhD '67) and Seung Ho Kim (PhD '66), have been recognized as Distinguished Alumni of the Department of Chemistry.





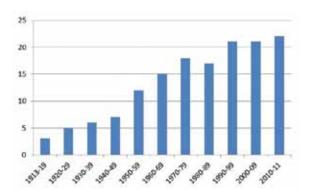
Chemistry Department History 3: Graduate Education

The Department has been awarding PhD degrees ▲ since 1913—almost a century! Within the next few years we will graduate our 1300th PhD student. Reading through the list of dissertation titles gives a sense of how chemical research has changed. For example, "The Formation of Utilizable Products from Natural Gas" by Roy Uhlinger (PhD '14) or "Theory of Distillation and the Laws of Henry and Raoult" by Ray Dunphy (PhD '15) are so broad that entire books have been written about these topics and they are deeply integrated into chemical technologies. While today's students work on very different topics, like their departmental ancestors they also work at the cutting edge of chemistry, gaining remarkable insight into complex chemical systems. (The list of dissertation titles makes interesting reading: www.chem.pitt. edu/sites/default/files/PHDLIST%2008%2011.pdf.)

Although the number of MS and PhD degrees fluctuates from year to year, the graph (below) shows a steady growth in our graduate program. Over the past decade, the averages are 22 PhD and 12 MS degrees per year. Our enrollment also fluctuates. It decreased through the 1990s, and has increased since then. The 20-year average is 193 graduate students. Today, there are over 200.

The first woman to receive a PhD from the Department was Rachel Kesler (PhD '26). Today, we have a graduate student population that is 31 percent female, (66/214) somewhat above the average for "large" graduate programs (ACS CPT report, Spring 2008).

Likely Edward Lee Harris was the first African American PhD in Chemistry at Pitt. Dr. Harris worked his way through graduate school as a Pitt custodian. After obtaining his PhD in 1937 under the direction of Professor Alexander Lowy, he went on to distinguish himself as a faculty member and chair at Wilberforce College and as a rocket fuels consultant to Wright-Patterson Air Force Base.



Many notables have graduated from the Department of Chemistry. A few are: Charles Glen King (MS '20, PhD '23, American biochemist noted for first isolating vitamin C); Paul Lauterbur (PhD '62, 2003 Nobel prize winner in medicine for his invention of magnetic resonance imaging); Abul Hussam (PhD '82; inventor of the Sono arsenic filter); Michael Strem (PhD '64; founder of Strem Chemicals); as well as numerous others.

The local chapter of the graduate student organization, Phi Lambda Upsilon (PLU), has played a key role in providing a rewarding graduate student experience. Beyond providing a social and professional network for graduate students, PLU is a key engine in two important departmental events, the biannual Alumni Awards ceremony and the Phillips Lectures. PLU organizes a roundtable discussion with our alumni awardees to provide an opportunity for oneon-one interaction between current graduate students and a few of their predecessors. PLU has actively contributed to the Department's scientific life through the Phillips Lectures. PLU has invited and hosted lecturers who are at the top of their field. In fact, the students have hosted nine Nobelists, eight before they received their prizes!

Our best students continue to compete effectively for fellowship support from within the University and beyond. In the last two years, graduate students have been awarded four Andrew Mellon fellowships, one ACS Division of Medicinal Chemistry fellowship, and one EPA fellowship. Because of financial resources made available through donors, friends, and alumni, the Department is able to bestow fellowships and awards; including Bayer MaterialScience fellowships and Goldblatt fellowships, which each include two semesters of support, as well as one semester fellowships (Kaufman, Braskem America, Inc., Clapp, and Safford) and travel grants (Strem).

Recent graduates have obtained postdoctoral appointments at top institutions (UC San Diego, Harvard, MIT, Scripps, Northwestern, U. Chicago), and have started careers at companies big and small. And of course many go on to teach the next generation of chemists.

We are proud of our legacy, as well as the high quality students in our program today.



PLU Officers: Brian Graham (co-president) Tim Cunninghan (co-president) Kristy Gogick (past president)

Erratum: Issue 7, Fall 2010, page 3, paragraph 1. "Chemistry Department History 2: On the Move – Our Commitment to Undergraduate Education". William Baldwin should be Wilmer E. Baldwin.



Department of Chemistry

Faculty 1971

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 Jeffrev. Professor

Kenneth Jeffrey Johnson, Asst. Professor

Frederick Kaufman, Professor

Robert Levine, Professor

Richard Hugh McCoy, Professor Dean and Director of Graduate Programs, Faculty of Arts and Sciences

Carolyn Wood Maricondi, Asst. Professor

Foil 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 1971: Where are they now?

In 1971, the Pittsburgh Pirates won the baseball World Series and the Children's Hospital of Pittsburgh created the iconic Mr. YukTM symbol. The Department of Chemistry published its first newsletter (www.chem.pitt.edu/newsletters/an71/an71.html) and conferred 31 PhD, 14 MSc, and 83 BSc degrees.

Lillian Schlosser Balchus (BS '71; Advisor: Chapman): Lillian is a chemist at Bayer Material Science.

Joseph G. Bubonic (MS '71 Forensic Chemistry): Mr. Bubonic began his career as a criminalist, performing drug, fire debris, and explosives analysis at the Pekin, IL satellite laboratory of the Illinois State Police Forensic Sciences Command in 1971. In 1973, he was named laboratory director. He married his wife, Debra, in 1973, and they have six children and five grandchildren. In 1985, he became a bureau chief at the central headquarters in Springfield, IL. Currently he is responsible for three of the regional laboratories. (jbubonic@juno.com)

Ellene Tratras Contis (MS '71): Dr. Contis has been at Eastern Michigan since 1971, where she has held various positions including director of the Women's Studies Program; Associate Dean, College of Arts and Sciences; and Associate Vice President for Academic Affairs. Dr. Contis is presently a professor of chemistry and project director of the Creative Scientific Inquiry Experience (CSIE) Program at Eastern Michigan University.

Geoffrey Dellenbaugh (PhD '71; Advisor: Douglas): Following his studies at Pitt, Dr. Dellenbaugh obtained a law degree from the University of Chicago and practiced patent and licensing law in the pharmaceutical and medical industry for 34 years. In 2008, he joined the University of Connecticut School of Law, where he co-teaches an intellectual property law clinic. Students under his direction provide free intellectual property law services (patents, trademarks, and copyright) to small businesses in Connecticut. (gdellenbaugh@cox.net)

James Eggler (PhD '71; Advisor: Danishefsky): Dr. Eggler retired from Pfizer in 2002, where he was a research advisor. (jfeggler@comcast.net)

Thomas B. Julian (BS '71; Advisor: Alfred Moyé): Thomas obtained his MD from the University of Pittsburgh School of Medicine in 1976. Presently he is the director of breast surgical oncology for the West Penn Allegheny Health System. In 2010, Dr. Julian received the Vivian and Meyer P. Potamkin Foundation Award for Breast Cancer Research. Other awards and distinctions include Pittsburgh Top Doctor (2010, 2011) and Pittsburgh Top Oncologist (2011). Dr. Julian was recognized as one of America's Most Compassionate Doctors in 2011. (T-julian@wpahs.org)

Eugene P. Mazzola (PhD '71; Advisors: Griffin, Cohen): Dr. Mazzola has headed the Nuclear Magnetic Resonance (NMR) Facility at the FDA's Bureau of Foods (later the Center for Food Safety and Applied Nutrition) since 1974 in Washington, DC. He was appointed an adjunct professor in the Department of Chemistry and Biochemistry at the University of Maryland and joined their shared NMR facility in 1997. His research program applies NMR to problems in organic and natural products chemistry. He has chaired the Washington Area NMR group since 1996, been a member of the organizing committee for the Small Molecule NMR Conference since its inception in 1999, and cochaired the meeting in 2004 and 2008. In 2008, Dr. Mazzola returned to the Department of Chemistry at Pitt to present both a workshop and a seminar on his NMR research. (emazzola@umd.edu; www.chem.umd.edu)

Arthur Nagel (PhD '71: Danishefsky): Dr. Nagel did his postdoctoral studies with Professor Ernest Wenkert at Indiana University. He worked for 30 years (1972-2002) at Pfizer Central Research (Groton, CT), where he was a research advisor. He and his collaborators are well known for the development of Geodon which is a novel atypical antipsychotic for the treatment of schizophrenia. Because of this discovery, Dr. Nagel was awarded the ACS Regional Industrial Innovation Award in 2005 and the ACS Hero of Chemistry Award in 2007. (anagel@comcast.net)

Michael Nardi (BS '71, MS '72 from the Graduate School of Public Health): After receiving his MS, Michael joined the research laboratory of Dr. Sandra Kaplan in the Department of Medicine at the University of Pittsburgh investigating white cell functions in patients with sickle cell disease. In 1978 he moved to the NYU School of Medicine where he is presently an associate professor of pediatrics and pathology. His academic endeavors in the fields of platelet immunology and laboratory diagnosis of hemoglobinophathies and thrombophilia are described in more than 70 publications. His clinical responsibilities include management of the Langone Medical Center Special Coagulation Laboratory. (michael.nardi@nyumc.org)



Larry Robert Needs (MS '71): Mr. Needs retired from the US Army in 1982. He went on to work for Hercules, Inc. (Wilmington, DE) and retired in 1995. From 1995-2000, he was general manager for European Racing Technologies. From 2001-2009 he was the dean of students and a chemistry teacher at the Christian Academy in Brookhaven, PA. He is now retired. (Isneeds@verizon.net)

Mark D. Stolorow (MS '71; Advisor: Tabor): Mr. Stolorow is currently director of the Law Enforcement Standards Office at the National Institute of Standards and Technology (NIST). (markgails@hotmail.com)

George E. Von Nieda (PhD '71; Advisor: Straub): Dr. Von Nieda is an environmental safety and health officer at the Los Alamos National Laboratory (Los Alamos, NM). He is currently working on safety issues with high explosives and homeland security. (vonnge@lanl.gov)



Alumni Updates

Ben Askew (PhD '88): Dr. Askew has joined Third Rock Ventures as an Entrepreneur-in-Residence (www. thirdrockventures.com.). Third Rock Ventures is a venture capital firm founded in 2007 with the mission of launching transformative life sciences companies.

Justin Chalker (BS '06): Justin gave a seminar this summer in the Department, and he expects to receive a PhD from the University of Oxford this fall.

Vincent Donnelly (PhD '77): Dr. Donnelly, the John and Rebecca Moores Professor at the University of Houston, received this year's AVS Thornton Award for "innovation of surface and plasma diagnostics to evaluate the complex kinetics of plasma processing, and for the development of fundamental reaction mechanisms to explain the complexity" (www2.avs.org/symposium/AVS58/pages/majawards.html). Vincent Donnelly is a faculty member in the Department of Chemical and Biomolecular Engineering.

Jay Jarvis (MS '79, Forensic Chemistry): After graduation, Mr. Jarvis worked for the Georgia State Crime Laboratory. In 2011, he retired after 32 years of service.

Peter Larkin (PhD '91; Advisor: Asher): Peter is working in the QbD analytical group at Pfizer in Groton CT. Recently, he authored a book entitled *IR and Raman Spectroscopy, Principles and Spectral Interpretation*. Elsevier is the publisher.

Edward Narke (BS '92): Ed is beginning his third year as principal and head of Regulatory Affairs for Design Space Inpharmatics (DSI), a chemistry, manufacturing, and controls regulatory consultancy firm.

Amit Paul (PhD '08; Advisor: Waldeck): Dr. Paul was recently hired as an assistant professor at the Indian Institute of Science Education and Research (IISER) Bhopal, India.

Lee Spangler (PhD '85): Dr. Spangler is the director of the Big Sky Carbon Sequestration Partnership and the Zero Emissions Research and Technology (ZERT) Center, which is a collaborative of DOE labs and academic institutions focused on the basic science issues underlying geologic carbon sequestration (see www.bigskyco2.org/about/staff).

Michael E. Strem (PhD '65): Founder of Strem Chemicals, received the ACS Charles Lathrop Parsons Award, in 2011.

James Valentini (BS '72): James Valentini has been named interim dean of Columbia College. He was chair of the Department of Chemistry from 2005 until 2008 and is currently the director of Columbia's chemistry department undergraduate studies program.



Faculty Highlights: Sanford A. Asher

Chemistry Professor Sandy Asher and his group are developing new optical materials, technologies, and spectroscopy methods for a variety of uses ranging from fundamental studies of protein folding to the "stand-off" detection of explosives. They are pioneering the development of UV resonance Raman spectroscopy for insightful explorations of the reaction coordinates of important complex systems. The Asher group has pioneered the development of smart photonic crystal materials that self assemble into 2-D and 3-D periodic arrays and diffract light for use in chemical sensing.

Smart Photonic Crystal Materials

In addition to being beautiful, these smart materials function as chemical sensing devices in which periodic arrays of particles are embedded in smart hydrogels. These hydrogels change volume as their chemical environment changes. The resulting changes in particle array spacings change the diffracted wavelength, changing the visually evident vibrant color. Sensors are being developed for both clinically and environmentally important analytes. Applications include embedding glucose photonic crystal sensors in contact lenses in order to sense glucose in tear fluid. Since the glucose concentration in tears tracks that of blood, this enables the noninvasive continuous monitoring of glucose for people with diabetes mellitus. The rumor that members of the Asher group often cry about their research topics is untrue.

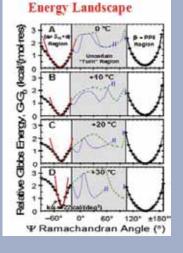


UV Resonance Raman Spectroscopy

The Asher group has pioneered the development of UV resonance Raman spectroscopy and developed it into a powerful technique for both fundamental and applied research applications. Raman scattering occurs when vibrational nuclear motion couples to the laser light induced polarization of a molecule's electron cloud. The generated Raman scattered light frequency results from the coupled oscillation at v_o - v_v , where v_o is the exciting light frequency and v_v is the molecular vibrational frequency. Resonance Raman excitation occurs when v_o occurs within an electronic absorption band. The resulting large induced dipole generates extraordinarily large Raman band intensities for particular vibrations, enabling high spectral sensitivities and high selectivities for specific chromophoric groups in the sample. The Raman spectra are very sensitive to molecular structure because the intensities are determined by the coupling of electromagnetic radiation to the electron cloud, and the coupling between electron cloud motion and vibrational motion.

Researchers in Prof. Asher's group constructed the first deep UV Raman spectrometers, which required them to work with laser companies to build deep UV lasers (190-250 nm). The deep UV spectral region contains numerous electronic transitions of molecular functional groups and this new technology has allowed the Asher group to develop an understanding of resonance Raman enhancement in both small and large molecules. They have demonstrated how to use these methods to study peptide and protein secondary structure in solution. They have also developed a way to monitor the Ramachandran Ψ dihedral angle of the peptide bond which lies along the most important protein folding reaction coordinate. This procedure allows them to determine protein and peptide secondary structure as well as the crucial Gibbs free energy along this reaction coordinate. These types of Raman studies are the first experimental approach capable of determining folding energy landscapes. They have also made possible the examination of the evolution of protein conformation in response to nanosecond and T-jump excitation that causes conformational melting.

In other studies, Asher group members are developing novel, handheld UV Raman spectroscopic instruments that excite distant surfaces with deep UV laser light and capture the backscattered light to monitor the resonance Raman spectra to detect explosives and other dangerous chemical species.







Faculty Nuggets

Kay Brummond was elected to the 2010 class of fellows of the American Chemical Society. Kay was also honored with a visiting professorship position at the Université Pierre et Marie Curie-Paris 6, Paris, France, and she has received a Visiting Fellow Award from the University of New South Wales in Australia.

Toby Chapman was inducted as a distinguished member of the University of Pittsburgh Chapter of the National Society of Collegiate Scholars for the academic year 2010-2011.

Dennis Curran (PI) was awarded a NIH Shared Instrumentation Grant to obtain a new state-of-the-art single-crystal X-ray diffractometer with a copper micro-focus X-ray source.

Billy Day is the 2011-2012 chairperson-elect of the steering committee of the Chemistry in Cancer Research working group (CICR) of the American Association for Cancer Research.

Paul Floreancig is featured in the 'Author Profile' section of the September 5 issue (Vol. 50, Issue 37) of *Angewandte Chemie International Edition*.

Geoffrey Hutchison's research was the featured "cover" for *J. Phys. Chem.* The Hutchison research group surveyed over 90,000 possible pi-conjugated co-polymers for organic solar cells, and discovered many with over 10% efficiency, well beyond the current experimental efficiency record. The paper highlights an efficient way to screen polymer solar cell materials. It also summarizes new design rules for synthesis.

Ken Jordan is part of a research team that received a highly competitive 2011 INCITE (Innovative and Novel Computational Impact on Theory and Experiment) Award.

Kaz Koide's collaborative resveratrol research was cited in Newsweek magazine.

Haitao Liu was selected by the New York Academy of Sciences to receive the 2010 Blavatnik Award for Young Scientists.

Michelle Ward Muscatello was awarded the J. Kevin Scanlon Award for the Promotion of Science by The Spectroscopy Society of Pittsburgh.

David W. Pratt was honored for his outstanding career as an educator, mentor, and research scientist in the September 1, 2011 issue of *The Journal of Physical Chemistry A*. The journal includes highlights of Dr. Pratt's career, tributes from students, and articles authored by faculty colleagues.

Renã Robinson was named the faculty advisor for the newly formed Pittsburgh chapter of the National Organization of Black Chemists and Chemical Engineers (NOBCChE).

Nat Rosi is a PI on a multi-institutional MURI (Multidisciplinary University Research Initiative) award from the Air Force Office of Scientific Research.

Sunil Saxena (PI) was the recipient of a \$1.62 million NIH Grants Award for a State-of-the-Art High Frequency Pulsed Electron Spin Resonance Spectrometer.

Alexander Star was awarded a 2011 Chancellor's Distinguished Research Award, and he was selected to receive a five-year National Institute of Environmental Health Sciences (NIEHS) Outstanding New Environmental Scientist (ONES) Award for his project, "Investigations and Mitigation of Carbon Nanomaterial Toxicity". Alex was also highlighted in the *Pittsburgh Post Gazette* (Pitt Chemistry Professor at the Forefront of a Futuristic Science).

Michael Trakselis was selected to receive a Research Scholar Grant from the American Cancer Society to support research on the "Mechanism of DNA Polymerase Switching During Replication to Bypass Lesions".

David Waldeck was elected to chair the Donor-Acceptor Gordon Conference in 2014.

Peter Wipf was elected to the 2010 class of Fellows of the American Chemical Society.



Graduate Awards

Andrew Mellon Predoctoral Fellowship Xing Yin Hong Zhang

Goldblatt Fellowship
Andrey Solovyev

Kenneth P. Dietrich School of Arts and Sciences Fellowships

Anthony Bencivenga
Liming Cao
Benjamin Eyer
Timothy McFadden
Sean Gardner
Liqing Gu
Wentao Jiang
Chong Liu
Hao Lu
Madu Mendis
Michael Nardone
Yangguang Ou
Brandon Parks
William Smith
Sijia Wang

Bayer Materials Science Fellowship

Adam Gagorik Yanan Chen Hyo Jeong Kim

Warga Fellowship Kristine Danowski Paula Hoffmann

Bayer Fellowship
Tyler Rohrs

Kaufman Fellowship Nathan Tavenor

Provost's Fellowship Zhe Ren Wanji Seo

Braskem America, Inc. Fellowship Jerry Caligiure



Graduate Highlights: Chad Shade

Chad Shade (BS 2005, PhD 2011) performed his thesis work under the guidance of Stéphane Petoud and examined the energy transfer from organic/semiconductor antennae to luminescent lanthanide

cations. During his time at Pitt, Chad received the Safford Teaching Award, the Teaching Assistant Mentorship Award, and he served as PLU president. He also gave a presentation entitled "Carbon Nanotubes Decorated with Dendrimer-Lanthanide Complexes with Unique Room Temperature O_2 Sensitivity" at Pittcon 2010 in Orlando Florida, based on work which was published in collaboration with the Star group (Nature Chemistry 1 (2009), 500).

Chad's thesis is entitled "Lanthanide-Containing Nanomaterials and Complexes: Utilizing Lanthanide Luminescence for a Broad Range of Application". His experimental studies of the antenna effect explored the use of several luminescent systems, including semiconductor nanocrystals, dendrimers, metal-organic frameworks, and micelles for developing biologic imaging agents and chemical sensors. These studies demonstrated the advantages of incorporating luminescent lanthanides within sub 5 nm host materials, a length scale where many fundamental biological interactions take place. Chad's later studies of the dendrimer-lanthanide complex laid



the groundwork for exploring the increased photostability of organic chromophores in the presence of suitably matched lanthanide cations. They were performed in the context of an *in vivo* colorectal metastatic cancer rat model.

Because of his long-standing interest in an academic career, Chad was frequently present in the undergraduate teaching office. During his first semester in the program, he was a teaching assistant for the general chemistry course and he was a teaching/laboratory assistant for Chem 0910: Chemistry for the Health Related Professions. Later Chad revised the eighth edition of the Chem 0910 lab manual with his long-time teaching mentor and friend George Bandik. Throughout his time in the Department, Chad participated regularly in the Chemistry Olympics and Saturday Science programs.

This past winter Chad accepted a postdoctoral position in the Mirkin group at Northwestern University, where he continues to draw upon the excellent experiences he had in Pittsburgh.

Phi Lambda Upsilon (PLU)

Phi Lambda Upsilon (PLU) is the National Honorary Chemistry Society founded in 1899 at the University of Illinois. The aims and purpose of the society are the promotion of high scholarship and original investigation in all branches of pure and applied chemistry. The University of Pittsburgh Xi Chapter has been affiliated with the National PLU since its charter in 1917.

In the 2010-2011 year, PLU sponsored and participated in a variety of activities. Notably, PLU sponsored a roundtable discussion with the 2010 Distinguished Alumni Awardees. PLU also organized the annual Francis Clifford Phillips Lecture. The 56th Phillips Lecture speaker, Dr. Michael Bowers of the University of California – Santa Barbara was selected for the inaugural lecture for the division of biological chemistry. Professor Bower's research has focused in part on the experimental and theoretical models of gas-phase structures of biomolecules. The titles of his talks were "The General Mechanism of Peptide Aggregation and Assembly: What Matters and What Doesn't" and "Amyloid Assembly and Oligomer Structure in Alzheimer's Disease, Parkinson's Disease and Type 2 Diabetes."

Social events sponsored by PLU include bowling, happy hours, Pirate games, and the holiday party. PLU also holds the annual first-year picnic outside on the first floor patio.

PLU ended the 2010-2011 year by initiating sixteen new members into the society in June. For more information on PLU, find us on Facebook (PluPitt), at our Web site (www.pitt.edu/~plu) or e-mail us at plu@pitt.edu. PLU officers for the 2011-2012 year are Tim Cunningham and Brian Graham (Copresidents), Mackenzie Speer (secretary), Marshall McGoff (treasurer), and Brandon Mills (media coordinator).

Undergraduate Spotlight: Jordan Deaner

Jordan Deaner graduated this past April with his Bachelor of Science degree, with a bioscience option, and both University and departmental honors. As an undergraduate, Jordan received several departmental awards including being corecipient of the 2011 Phillips Medal given to the highest ranking graduate. Jordan (right in picture below), shared this award with Christopher Hughes (left in picture below). (Christopher is



currently working for the Teach for America Program in Arizona.) As an undergraduate, Jordan was active as a peer leader for several faculty members teaching organic chemistry and was also a laboratory instructor for the honors organic laboratory class. He carried out undergraduate research under the direction of Professor Dennis Curran where he investigated the chemistry of N-heterocylic carbene boranes. Jordan also found time to give back to the community as a co-outreach coordinator with our ACS-SA. Jordan spent time working with young people at St. Agnes School in Oakland, and Good Shepherd School in Braddock, as well as many young visitors to the Department. Like so many of our undergraduates, Jordan fully gave of his own time to help others succeed, while also finding time to succeed academically. Jordan is currently pursuing his MD degree at Jefferson Medical College in Philadelphia.

We are grateful to all of our undergraduates who make the Department of Chemistry a very special place.

ACS Student Affiliate News

he ACS-SA is an important part of the undergraduate chemistry community at the University of Pittsburgh. Through speakers, outreach efforts, and social programming, the group maintains a presence on campus and shares its enthusiasm for chemistry and science with others. The ACS-SA has established a tradition for involvement and strong leadership on campus and in the community. The ACS group is special because it reaches out to more than just undergraduate chemistry majors. We have members majoring in subjects that range from neuroscience and biology, to psychology and history. Even though members have varied backgrounds and interests, we find that participants share a deep commitment to volunteering, community outreach, tutoring, and mentoring.

This year, we plan to expand our undergraduate mentoring program. In this program, an upperclassman "adopts" an underclassman and provides advice for succeeding at the University. The program was successfully piloted last year, and we believe a good goal for this coming year is to get more students involved. This program fosters relationships between students at different stages of the program. Strengthening ties within the Department of Chemistry, as well as to other related facets of student life, gives our students a strong support system within the chemistry community. We anticipate that the relationships young students form with upper class students will encourage and foster their interests in entering the sciences.

We plan to maintain our well-established reputation for environmental awareness and outreach within the community. The group has consistently been recognized for green chemistry efforts. We look forward to bringing in speakers from environmentally aware industrial companies and continuing our green chemistry newsletter updates. In addition, the group participates in various outreach programs, including National Chemistry Week, Saturday Science, and Chemistry Olympics. Over the years, the ACS-SA Chapter has found that members are thrilled to participate in these outreach efforts and community programs.

2011 Undergraduate Senior Awards

The American Institute of Chemists Award

Nathaniel A. Pancoast

The Mary Louise
Theodore Prize
Evan J. Carder
Elizabeth A. Gilji
Elizabeth C. Hocking
Chelise M. Hottel
Eric E. Peterson
Samantha K. Tieszen

The Merck Award
Lauren E. Campbell
Kaitlyn S. Musco

The SACP College Award
James J. Cregg

The Silverman Prize Sonya M. Bohaczuk

*The Phillips Medal*Jordan D. Deaner
Christopher P. Hughes

Department Milestones

RETIREMENTS: David W. Pratt (10/68-8/2011)

On Friday September 16, 2011, Dr. David W. Pratt was honored on the occasion of his retirement from the Department of Chemistry after more than 40 years of service. To a standing room only audience in the Ashe

Auditorium, Professor Pratt gave a talk relating his "Adventures in High Resolution Spectroscopy". Current and former students, faculty colleagues, and friends enjoyed the presentation, as David highlighted his group's recent research developments in his own enthusiastic inimitable style. A reception followed in the University Club ballroom.

A native of Rhode Island, David received his bachelor's degree from Princeton University, followed by a tour of duty in the U.S. Navy. After completing his PhD in chemistry at the University of California, Berkeley, he spent time as a postdoctoral associate at UC, Santa Barbara. David joined the faculty at the



University of Pittsburgh in 1968; in 1978 he was promoted to full professor. He has received numerous awards throughout his career, including a Fulbright Fellowship in 1979, Guggenheim Fellowship in 1985, Chancellor's Distinguished Teaching Award in 1994, the Earle K. Plyler Prize for Molecular Spectroscopy in 1999, Chancellor's Distinguished Research Award in 2001 and the Pittsburgh Award of the ACSociety in 2005. Most recently, in the September 1, 2011 issue of *The Journal of Physical Chemistry A*, David was honored for his outstanding career as an educator, mentor, and research scientist. The publication included tributes from students and articles authored by David's faculty colleagues.

The Department of Chemistry extends its congratulations and best wishes to David and Kathleen.

New Faculty

Sean Garrett-Roe, Assistant Professor

Dr. Sean Garrett-Roe comes to the Department from a postdoctoral position in Professor Peter Hamm's group at the University of Zurich, Switzerland where he developed a new ultrafast nonlinear infrared spectroscopy (3D-IR) technique that was awarded the 2009 Editors Choice Award by the Journal of Chemical Physics. This

technique has revealed heterogeneous dynamics in hydrogen bonding in ambient water. Sean was awarded his PhD in Chemistry from the University of California, Berkeley for his work on theoretical and experimental techniques to understand electron dynamics at the interface between a metal surface and a thin molecular film. He received his undergraduate degree in chemistry from Princeton University in 1999.

Dr. Garrett-Roe's research at the University of Pittsburgh will focus on the development of multidimensional IR techniques (2D and 3D) to study ion uptake and selectivity in a variety of systems, including ion channels, ion sensors, and ionophores. He has published 23 refereed papers.



Jill E. Millstone, Assistant Professor

Professor Jill Millstone comes to the Department from the University of California at Berkeley where she completed her postdoctoral work studying organic-inorganic hybrid photovoltaics in the group of Jean M.

J. Frèchet. She received her undergraduate degree in both Chemistry and English, from Carnegie Mellon University in 2003. In the same year, she moved to Northwestern University to carry out her PhD research on the synthesis and application of anisotropic nanoparticles under the direction of Chad A. Mirkin.

Her current research focuses on the study of nanostructure surface architectures, with the goal of developing highly tailored materials for use in medical devices and alternative energy systems. Dr. Millstone has 22 publications as well as a US Patent, and she has submitted five additional patent applications.





Bhaskar Godugu (Mass Spec)

Dr. Godugu has joined the Department of Chemistry as a research assistant professor and director of the Department's Mass Spectrometry facility. Bhaskar was awarded his PhD in Organic Mass Spectrometry

etry from the National Center for Mass Spectrometry, Indian Institute of Chemical Technology (IICT), Hyderabad, India. He performed his post-doctoral research work at the Mass Spectral Data Center in the National Institute of Standards and Technology (NIST). He mainly focused on spectrum repeatability and reproducibility under different experimental and instrumental conditions, such as temperature, pH, digestion times, spray voltage, etc. by using digested protein solutions. His research involved mass spectral studies of biologically important compounds and their interaction with cations and anions using soft ionization techniques.



His current research interests include peptide chemistry; peptide fragmentation studies on different instruments and interactions of metal ions and biological molecules in the gas phase, as well as metal ion binding strengths of biological molecules.

Carol Fortney, Lecturer

Dr. Carol Fortney earned undergraduate degrees in Psychology and in Chemistry from the University of Pittsburgh. Carol also completed her graduate work at the University of Pittsburgh under the direction of the late Professor Rex Shepherd, and under the direction of Professor Emeritus Bodie Douglas. As a graduate

student researcher, Carol published two papers on the development of ruthenium nitrosyl compounds for use as nitric oxide delivery agents. As a graduate student teaching assistant under Dr. George Bandik, Carol taught and coordinated the Organic Chemistry I and Organic Chemistry II labs and trained graduate student teaching assistants within the Department of Chemistry, as well as through the University of Pittsburgh's New Teaching Assistant Orientation. Carol received the Safford Award for Excellence as a graduate student teacher in 2001. Since completing her graduate work in 2007, Carol has served as a general chemistry visiting lecturer,



temporary coordinator of the undergraduate Analytical Lab Program, and as an assistant to Dr. Ericka Huston who directs the undergraduate Organic Lab Program. In November of 2007 Carol was awarded the Greek Life Scholarship Award for Excellence in Teaching. This year Carol is teaching General Chemistry I and General Chemistry II while assisting Dr. Huston with the organic lab program.

Susan Maleckar, Lecturer

Dr. Susan Maleckar, formerly Susan Dally, was recently named a lecturer in the Department. She is a native of Butler, Pa., and completed her undergraduate degree in chemistry at Geneva College. Susan received her PhD from the University of Pittsburgh under the direction of Professor Toby Chapman. She has taught at the University of Pittsburgh as a visiting lecturer for the past seven years and will continue teaching engineering chemistry, general chemistry, and organic chemistry. Her interests include chemistry education and outreach, and she continues to be involved in the Chemistry Olympics. Susan's previous awards include the Safford Award for Excellence in Graduate Teaching.





Diversity initiatives in the Department

The Department of Chemistry recognizes and values diversity, and we are committed to recruiting and retaining a diverse student body. This commitment is highlighted by the establishment of two organizations in 2010, the Pittsburgh Chapter of the National Organization of Black Chemists and Chemical Engineers (NOBCChE) and the Pittsburgh section of the American Chemical Society Women Chemists Committee (ACS-WCC).

NOBCChE's primary goal is to increase under-represented minority participation in science, math, engineering, and technology (STEM). This goal is achieved by providing members with opportunities to attend scientific seminars, regional and national conferences, chapter meetings, community outreach events (K-12), and professional development activities. Professor Renã Robinson is the Pittsburgh chapter's faculty advisor. (For additional information, send an email to pittsburgh.nobcche@gmail.com.)

The WCC's mission is to be a leader in attracting, developing, promoting, and advancing women in the chemical sciences. The organization is off to a running start having hosted a kick-off dinner at the Spaghetti Warehouse on September 29 and an "Empowering Women in Science Symposium" on November 5. Dr. Michelle Ward Muscatello is currently the chair of the Greater Pittsburgh WCC. Please see www.pitt.edu/~pghwcc for more information.

The Kenneth P. Dietrich School of Arts and Sciences and Department of Chemistry at the University of Pittsburgh sponsored a Committee on the Advancement of Women in Chemisrty (COACh) workshop (http://pages.uoregon.edu/coach/index.html) for tenure and non-tenure stream women on Saturday, October 1, 2011. The workshop, entitled "Basic Negotiations, Problem Solving and Conflict Resolution," was facilitated by Drs. Jane Tucker and Barbara Butterfield. The workshop is designed to build understanding of mutual-interest-based negotiations or solution finding and was attended by nearly 40 women science faculty from the Pittsburgh area.

The Department is proud to support these initiatives and encourages student and faculty involvement!







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A warm thank you to those who made donations from July 1, 2010-June 30, 2011

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If you would like to contribute, please visit our Web site at www.chem.pitt.edu or return the enclosed envelope. We appreciate your donation.



Renovation, Expansion, Modernization

The Department of Chemistry is being transformed to keep pace with changes in technology, to meet the needs of our graduate research programs, and to update our undergraduate laboratory experience. Newly renovated research lab space in Eberly and in Chevron, a computer classroom on the Ashe balcony, two floors of newly constructed research laboratories in the Chevron Annex, four modern undergraduate chemistry labs in Chevron, and an inviting entrance with space in which to relax, meet, or study. All of these changes aim to enhance education in chemistry for Pitt students now and into the future.

Extreme Makeover-Chemistry Edition has taken place on the second floor of Chevron. The undergraduate general chemistry labs in Chevron have always been somewhat unusual in design, combining both a recitation discussion area and lab bench space in a single room. A novel solution has allowed us to incorporate these combined recitation/lab areas into the modern design of our newly renovated labs. Lab benches occupy peripheral wall space. A flexible arrangement of tables and seating, adaptable for formal lecture presentations or small-group discussions, is located in the center of each room. This central core is separated from lab experiments by glass partitions, providing a safety barrier and excellent sightlines throughout the lab and enhancing opportunities for interactions among students and between students and lab instructors. The glass also serves as a writing surface for small-group instruction; while a traditional chalkboard is still located at the front of the room.

Lab work space includes both open lab benches (for "analytical" style lab exercises) and aircapture units (for "organic" synthesis and reactive chemistry activities), suitable for the variety of experiments conducted in our introductory lab courses. The new labs are equipped with a labtop PC for each student lab station, as well as an instructor PC connected to the room's projection system, enabling enhanced use of technology in the lab. The laptops are interfaced with temperature, pH, conductivity, and visible absorption spectrometers (Vernier electronic probes) that promise to change the way we teach and the way students experience chemistry. Practice with concepts and some pre-lab material utilize Excel spreadsheets, however we are planning the inclusion of electronic notebook software in the near future. Thus, bringing the whole experience into the digital age. As we gain familiarity, we will include video clips to illustrate lab techniques. Ultimately our students will have the capability to submit their lab reports electronically.

Chevron Annex construction has been completed and Prof. Peter Wipf's research group has begun to relocate into these bright up-to-date facilities. Perched above the Ashe auditoriums, the new space is connected to Chevron on the sixth and seventh floors.

What was once part of the Chemistry Library on the second floor in Eberly is now new labs and office space. The research labs on the fifth floor of Chevron have also been redone to match the open floor plan design that was recently introduced on the 14th floor.

The Chemistry Computer Classroom (C³), which now occupies the western end of the Ashe balcony, can accommodate 30 students, each with their own computer, for interactive classes, training programs, and study sessions.

The Cantini mural in the Ashe lobby now looks over a common area replete with tables, chairs, ottomans, and chalkboard wall space that has become a popular spot for students and faculty alike.

These are just some of the highlights of recent updates to Department of Chemistry facilities. Stay tuned for further improvements as the Department continues to advance its physical infrastructure!





Picture Captions

- 1 Chevron Science Center
- 2,3 Second floor undergraduate chemistry labs (CSC)
- 4 Fifth floor research labs (CSC)
- 5 Eberly Hall
- 6,7 Second floor research labs (Eberly)
- 8 Chevron Annex from patio
- 9,10,11 Sixth and seventh floor research areas of Annex
- 12 Chemistry Computer Classroom

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We look forward to hearing from you!

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