Greetings from the Chair

elcome to the fall 2013 issue of the Department of Chemistry Newsletter. While last year presented a number of fiscal challenges, the Department had a successful year in its mission activities of research, teaching, and service. Last year, the Department graduated 67 BSc, 9 MSc, and 21 PhD chemists. Currently, we have 267 declared chemistry majors in the undergraduate program, 212 students in the graduate program working toward their degrees, and 30 postdoctoral students.

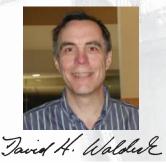
The Department has continued to grow its faculty to meet the instructional demands of a growing undergraduate population and to maintain leading research programs across a spectrum of modern chemistry's frontiers. This year the Department hired five new faculty: a full professor (Alex Deiters), an assistant professor (Kabirul Islam), a lecturer (Hannah Morris), and two instructors (Gregg Huston and Tamika Madison); see pages 10 and 11. These faculty bring important expertise in chemical biology and biological chemistry to the Department's research profile and perspectives, ranging from experiences in industrial chemistry to that in art conservation, to our teaching faculty. While the faces in the Department continue to change, the Department remains committed to excellence in research, teaching, and the mentoring of a new generation of chemists.

Improvements to the chemistry complex and the research and teaching infrastructure have continued, albeit at a somewhat slower pace over the last year. The major event over the past year is the opening of the Chemistry Instrumentation Center (CIC) which houses the Department's NMR, Mass Spectrometry, and X-Ray crystallography resources. This new space (see pages 14 to 15) integrates support activities for research, particularly small molecule efforts, and is available to trained students 24/7. The machine shop has been combined and moved across the street in its merger with the Physics machine shop. It has a strong staff of four people, is led by Tom Gasmire, and has much improved machining capabilities than in the past. The next major activities will be a complete renovation of research space on the thirteenth floor and the

Pelcome to the fall 2013 issue of the general chemistry labs on the first floor, which Department of Chemistry News- we hope to report on in next year's newsletter.

The Department plans to complete its strategic planning this academic year and has scheduled an external advisory committee to meet with us in the spring. 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 year time frame. As the faculty move through this process we may solicit your advice and input. We are grateful to those who have helped us already, and we hope that you will be generous with your time if we come to you over the next year.

A number of stories in this letter aim to introduce you to Department members and alumni. On page 2 we provide a collection of updates from the class of 1973, and on page 3, we provide short vignettes on the activities of two PhD alumni from the 1990's (Jane Valenta and Chris Miller). We provide additional updates on page 5. We hope that you will continue to share your activities with us through the newsletter or through our Facebook page, www.facebook.com/ pittchemdepartment. The activities of Professor Alex Star and his group's exciting work with carbon nanomaterials is highlighted on pages 6 to 7. Although we would like to introduce you to all of our newest alumni, this would be difficult, rather we provide a brief profile of an undergraduate and of a recent PhD graduate on pages 8 and 9. While the size of the Department's staff remains below that of the recent past, we have hired three new staff people since our last newsletter; see page 11. I hope that these and the other stories in this issue will provide you with some pleasurable reading. Finally, I wish to thank all of those who have contributed financially to the Department (see page 13). Your support plays an important part in helping us meet our mission.



DEPARTMENT OF CHEMISTRY UNIVERSITY OF PITTSBURGH
CHEVRON SCIENCE CENTER

Issue 10 2013

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University of Pittsburgh

Department of Chemistry

Faculty 1973

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

Bodie E. Douglas, Professor

Paul Dowd, Assoc. Professor

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

Lawrence M. Epstein, Assoc. Professor Dennis H. Finseth, Instructor

Henry S. Frank, Professor Paul Anthony Grieco, Asst. Professor

Klaus H. Hofmann, Professor and

Charles Alvin Hollingsworth, Professor

George Allen Jeffrey, Professor

Kenneth Jeffrey Johnson, Assoc. Professor

William Martin Kadunce, Instructor

Frederick Kaufman, Professor Robert Levine, Professor

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

Foil A. Miller, Professor and

Director, Spectroscopy Laboratory Alfred Leon Moyé, Assoc. Professor

David Wixon Pratt, Asst. Professor John Wayne Rabalais, Asst. Professor

V. Udaya Shankar Rao, Asst. Professor Gordon Alan Ryan, Asst. Professor

Hurd Winter Safford, Professor

Peter Emil Siska, Asst. Professor

Darel K. Straub, Assoc. Professor

Joseph J. Taber, Professor and Administratve Officer; Adjunct Professor, Dept. of Chemical and Petroleum Engineering



Class of 1973: Where are they now?

⁷n 1973, the Vietnam War ended, the Watergate scandal unfolded, and the OPEC Oil Embargo triggered the 1973 energy crisis. During this year, the World Trade Center officially opened, Federal Express Legan operations, and the Sears Tower in Chicago was finished. The Nobel Prize in chemistry was awarded to Ernst Otto Fischer and Geoffrey Wilkinson for organometallic chemistry. The Miami Dolphins had a perfect season; and the Pittsburgh Pirates' Roberto Clemente was inducted into the Baseball Hall of Fame. Skylab, the United States first space station was launched, and on December 28, the Comet Kohoutek, a long-period comet, was at perihelion. Its next apparition will be in about 75,000 years

Hedy Gruenebaum Abromovitz (BS '73; Advisor: Wallace): After a long career at Westinghouse Nuclear Energy Systems, Ms. Abromovitz now works as vice president of operations for PARLUX Fragrances, LLC. She is responsible for quality, package development, regulatory compliance, materials management, logistics and distribution for PARLUX, which manufactures fragrances for celebrities such as Rihanna, Vince Camuto, Marc Ecko, Jay-Z, Jessica Simpson, and Paris Hilton. Hedy is the coauthor of two books dealing with quality improvement and customer service. She and her husband divide their time between Pittsburgh and Boca Raton, Florida.

Robert DaRosso (BS '73): Dr. DaRosso is a physician and has been working at Beth Israel Medical Center in New York City as a Pediatric Hospitalist for 17 years. He has been married for 16 years to Marisol Lopez-DaRosso, and they have two children, Matthew and Daniel.

Dennis Finseth (MS '69, PhD '73; Advisor: Miller): Dr. Finseth worked for the Department of Energy for 25 years while also teaching part-time at Pitt. He was also a Pittsburgh high school teacher for seven years. Dennis recently moved to Michigan where he is a freshman seminar lecturer at the University of Michigan and an instructor of Organic/Biochemistry at Washtenaw Community College. He has two daughters and one granddaughter. (dhfins@gmail.com, finseth@umich.edu)

Edward C. Frese (BS '73; Advisor: Coetzee): Dr. Frese was employed at the Beaver Valley Power Station from 1973 until 1985. Since 1985 he has been employed at Dominion Resources, Inc. as a chemist providing technical support for Dominion's nuclear power stations. He plans a 2016 retirement.

Dr. Joyce Fehl Haskell (BS '72; Advisor: Miller): Retired. Dr. Haskell is a past District Governor of Lions Club International, and a past chairman of Storm Eye Research at the Medical University of South Carolina. Her husband is the Honorable A. C. Haskell, County Councilman for Aiken County, SC. They have three daughters and four grandchildren. (jhaskellgbd@yahoo.com)

Lester D. King (BS '73; Advisor: Safford): Dr. King is a member of the Authority Database Operations and contributed to the testing and development of the Structure Search Modules for SciFinder. He is married and his wife, Arna, works for the Journals Division of the American Chemical Society. They have two children and two grandchildren. (lesterking@hotmail.com)

Herbert Kloss (BS '73): Dr. Kloss is an anesthesiologist, as well as a jazz musician. His latest CD is entitled "Far From Home." (jazzgasman@hotmail.com)

Timothy Joseph Kross (BS '73): Dr. Kross is a physician and currently in private practice in the North Hills area of Pittsburgh; he specializes in internal medicine and addiction medicine. He has been married for 30 years and has three adult children. (drkrossmd@comcast.net)

Dorothy J. Menges (MS '73): After receiving her MSc in the Department's forensic chemistry program, Ms. Menges took a position at the Allegheny County Crime Laboratory, first as a chemist, and then a serologist and criminalist. In 1987, she became the manager of the Forensic Serology Laboratory at the Allegheny County Department of Laboratories. As a professional criminalist she makes appearances in criminal courts many times per year. Dorothy has also been active in teaching and mentoring through the Allegheny Police Academy, CCAC, and the University of Pittsburgh. She and her husband have two children.

John Nakovich Jr. (PhD '73; Advisor: Miller): After 33 years of service, Dr. Nakovich retired from the CIA in 2010. He has been married for 38 years and has a son and daughter. Both of his children are graduates of Virginia Tech. (nakojohn@aol.com)

George Plummer (BS '73): Dr. Plummer was a regulatory director at Siemens Healthcare Diagnostics until his retirement in October 2012.

University of Pittsburgh

Alumni Vignettes:

president for environment, health, and safety at PPG.



ane Valenta (MSc 1987, PhD 1994) has been the associate director for performance coatings R&D at PPG, Inc. since 2008. In her position, Jane is responsible for early-stage product research of Automotive Refinish and Protective & Marine Coatings. Jane's team at the Coatings Innovation Center in Allison Park, Pa. is part of a global organization involved in all stages of coatings research and product development.

After earning her MS degree in chemistry from the University in 1987, Jane joined PPG's business training program and quickly moved into product development and analytical chemistry. In 1993, PPG granted her an education leave to complete her PhD dissertation (Weber, 1994). She returned to PPG in

1994 in product development and progressed from being an individual contributor to being a project leader and then to group leader in Automotive OEM and Automotive Refinish before being appointed to her current position in 2008. As of December 1, Jane will be taking on a new role as vice

Jane's success and satisfaction stems from her ability to balance work and her personal life. Reflecting on her career over the past 25 years she stated: "I have been fortunate to work for a company that provides flexibility when I need it while also having a strong family support system that understands the demands of my position."



r. Chris P. Miller (PhD 1993) earned his PhD in chemistry from the University of Pittsburgh under the guidance of Professor Peter Wipf. After graduation, Chris went directly to work in the pharmaceutical industry as a medicinal chemist at Wyeth Pharmaceuticals (now Pfizer). While at Wyeth, Chris led the chemistry side of numerous drug discovery efforts, and he was responsible for the introduction of several compounds into human clinical trials. His research accomplishments include the invention of the drug bazedoxifene, a selective estrogen (approved by the FDA on October 3, 2013), both as a drug monotherapy for osteoporosis as well as a combination product for the treatment of menopausal symptoms. The bazedoxifene patent was the winner of a 2006 Thomas Alva Edison patent award. Chris has dozens of patents

and scientific publications to his name. Chris credits much of his growth as a scientist to his time in the Department, "... the most formative and productive years in my development as a chemist and also as a scientist!"

In addition to medicinal chemistry and drug discovery, Chris is interested in patent law, and obtained a JD from Temple University in 2001. He recently coauthored a chemistry patent law text, *The Chemist's Companion Guide to Patent Law*, with fellow researcher Dr. Mark Evans.

Alumni Updates

Andrew Bartko (BSc '87; Advisor: Waldeck): After receiving a PhD in chemistry from Georgia Tech, Andy did a postdoc and then took a position at the Batelle Memorial Institute, where he is a principal investigator and program director for technology development.

Anthony Bencivenga (MS '13; Advisor: Nelson) is employed at Allergan Bioscience Labs in Irvine, Calif.

M. Bhupathy (PhD '85; Advisor: Cohen) is the Executive Director of the pharmaceutical company Amgen.

Laura Borland (PhD '05; Advisor: Michael): In March 2013, Dr. Borland joined DuPont Central Research and Development, in Wilmington, DE as the communications manager. She leads the development and implementation of the internal integrated communications plan for CR&D in support of DuPont's Science and Technology. Previously, she spent five years as a chemical, biological, and explosives consultant with Booz Allen Hamilton.

John P. Cherkauskas Jr (PhD '93; Advisor: Cohen) is the vice president of global fragrance research at International Flavors & Fragrances.

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CALL FOR NOMINATIONS

The Department is soliciting nominations for the 2014 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, industry, volunteer efforts, or other significant contributions to society.

Nominations should include:

- 1. Your nominating letter
- 2. From one to 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.

For full consideration,
nominations should be mailed by
January 15, 2014
to:
Assistant Chair
Dept. of Chemistry
University of Pittsburgh
Pittsburgh, PA 15260



Alumni Updates (continued)

James E. Copenhafer (PhD '06; Advisor: Meyer): After a one-year postdoctoral position at Arkema, Dr. Copenhafer joined INVISTA in 2007. INVISTA is the world's largest integrated fiber, resin, and intermediates company. Their products include Lycra® fiber, and Stainmaster® carpeting, among many others. After several years as an R&D research chemist, Dr. Copenhafer transitioned to a position as an intellectual property liaison. He is now pursuing a degree in patent law at Widener University School of Law.

Slava Fishman (PhD '00; Advisor: Grabowski): Since graduation from Pitt, Slava has worked as a senior research specialist at the Environmental Analytical Laboratory for Dow in Midland, Michigan. His research and professional interests include development and application of novel mass spectrometric and analytical concepts to support various R&D engineering experiments, to improve waste treatment and process monitoring operations, to implement pollution source-finding in large integrated plant sites, and to demonstrate compliance with existing guidelines. He has been married to Lyuba for 22 years and they have three boys.

Amanda L. Garner (PhD '08; Advisor Koide): This fall, Dr. Garner took a new position as an assistant professor in the Department of Medicinal Chemistry at the University of Michigan, Ann Arbor.

Maryll Geherty (PhD '13; Advisor: Nelson): Maryll recently began a postdoc position at Princeton University. with Prof. Erik Sorenson.

Binbin Guo (PhD '13; Advisor: Nelson): Binbin recently took a position at Lubrizol Corp.

James Hale (PhD '12; Advisor: Nelson): James recently took a position at Knopp Bioscience.

Claudia B. Jaffe (formerly Claudia B. Cohen) (PhD '93; Advisor: Weber) is a cofounder and serves as executive vice president of business development at Lumencor, Inc. in Beaverton, Oregon. She has developed, published, and patented a variety of electrochemical and photoelectrochemical sensors and bioanalytical chips, focusing on high throughput analyses in enzymology, immunology, and genomics. Before Lumencor, she worked at Caliper Technologies, Protogene Labs, Agilent Technologies, and Quantum Vision. Dr. Jaffe is an inventor on numerous company patents, identifies new product development and business opportunities, creates all marketing collateral, and manages the sales team.

Lei Liu (PhD '11; Advisor: Floreancig): Dr. Liu is currently a professor at Shandong University in Jinan, China.

Dennis McCullough (PhD '88; Advisor: Cohen): Formerly senior vice president of the Advanced Resins Division at Bayer Material Science, Dennis is now vice president at Synthomer, for South East Asia.

Branko Mitasev (PhD '06; Advisor: Brummond): Branko currently works at Eisai Inc. in Andover Massachusetts, where he is part of the Pharmaceutical Science and Technology unit. As a CMC team manager, he oversees a global multifunctional team of scientists responsible for process development and manufacturing of drug candidates to support toxicology studies, regulatory filings, and clinical trials. Branko is married to Barbara Serli, who was also a researcher in the Department, and they have two children, Alexander and Bianca.

Andrew Napper (PhD '02; Advisor: Waldeck): Dr. Napper was recently promoted from associate professor to professor of natural sciences at Shawnee State University in Ohio.

Mark Schraf (BS '85): Mark graduated from WVU in 1990 with a MSc in analytical chemistry. After working for nine years in industry, he returned to WVU in 1999, and he has been teaching freshman chemistry there ever since, receiving a number of teaching awards. Mark is also a sportswriter for The Dominion Post in Morgantown, an author (*Cooperstown Verses: Poems About Each Hall of Famer*; McFarland, 2001), and fiction editor of SPITBALL: The Literary Baseball Magazine. Mark has been married for 22 years to Jeanne; they have a son Zach, 15, and a daughter Kaylee, 13.

Katherine Stone (PhD '09; Advisor: Saxena): Katherine is currently a research scientist in the Product Development group at Pacira Pharmaceuticals in San Diego, CA. Her work focuses on formulation development, pharmacokinetics, and the release characteristics of drugs encapsulated in DepoFoam, Pacira's proprietary multivesicular liposomes. DepoFoam provides the extended release of drugs and is the platform for the newly marketed local analgesic, Exparel.

Thomas Vargo (PhD '11; Advisor: Nelson): Thomas is employed at AbbVie Pharmaceuticals.

Feng Wang (PhD '03; Advisor: Jordan): Dr. Wang moved from Boston University and is now an associate professor in the Department of Chemistry and Biochemistry at the University of Arkansas.

Jianjun Wei (PhD: '04; Advisor: Waldeck): Jianjun recently left CFD Research Corporation and took a position as an associate professor at the Joint School of Nanoscience and Nanoengineering in North Carolina. (http://jsnn.ncat.uncg.edu/faculty/jianjun-wei-ph-d/)

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Remember that you can visit the Department of Chemistry Facebook page

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Chemistry Department History 5: Chairmen in the First Seventy-Five Years

Population of Francis Clifford Phillips to the University faculty. Over the next seventy-five years, the Department grew from a faculty of one and a handful of undergraduate students to a major research Department with over twenty faculty and hundreds of BSc, MSc, and PhD alumni.

Phillips was chair of the Department for forty years and guided it through many challenges and significant growth. During his tenure, the University relocated three times before settling in the Oakland neighborhood and many of these moves involved significant investments in laboratory space for chemistry instruction and teaching. During his first five years the Department had seven bachelor's graduates and no MSc or PhD programs, but during the last five years of his tenure the Department conferred nineteen Bachelor's degrees, ten Master's degrees, and eight PhDs. He also played an important role in opening learning opportunities for women in chemistry and in the creation of the Pittsburgh Chapter of the American Chemical Society. Phillips played an important role in establishing a city water filtration plant, which ended a series of typhoid epidemics that killed hundreds of Pittsburghers. In addition, Professor Francis Clifford Phillips gained an international reputation for his research related to petroleum and natural gas and in the analysis of steel. During his tenure, many of his students took important positions in industry, and he laid the groundwork for the Department's growth as a center of teaching and research.

Upon Phillips' retirement in the fall of 1915, the School of Chemistry was created with Raymond Bacon as the Dean. Bacon was also the director of the Mellon Institute, which had been founded in 1913. In 1918 Alexander Silverman was appointed Dean of the School of Chemistry. While this period was brief it laid strong ties between the Department and the Mellon Institute that were important to the Department's research profile over the next fifty years. In fact, many PhD students performed their research with Mellon Institute scientists, including Paul Lauterbur (PhD 1962) who won the 2003 Nobel Prize. In addition, many Mellon Institute scientists contributed to the Department's teaching mission. This relationship lasted until 1968 when the Mellon Institute ceased to exist as an independent entity.

In 1920, the University converted the School of Chemistry back to a Department and appointed Alexander Silverman as the head. Silverman was a graduate of the University (PhB 1902; MSc 1907) and was awarded the honorary ScD from the University in 1930. Silverman led the Department in this capacity until 1951. The world experienced epic changes during these decades, and they had a significant impact on the University and the Department. During this time the Department's research profile grew and broadened significantly with a number of notable faculty; including C. G. King (noted for his work in isolating Vitamin C and in nutrition chemistry); Klaus Hofmann (noted bioorganic chemist), Alexander Lowy (organic chemistry), and W. E. Wallace (magnetic materials and physical chemistry) among others. Extramural funding of research began in earnest during Silverman's chairmanship. Funding for research came from companies (e.g., Abbot Laboratories, Ciba Pharmaceuticals, Hoffman LaRoche, Parke-Davis, Swift, and Wheatena among others), from government contracts (Office of Scientific Research and Development (WWII), National Defense Research Committee, Office of Quartermaster General, and US Public Health Service), and foundations and organizations (Carnegie Inst., National Research Council, Nutrition Foundation, Research Corporation, and the Buhl Foundation). Support from the Buhl Foundation, which began in 1936, was especially critical for the Department, because it provided significant and sustained funding for more than a decade that allowed the infrastructure for research to be created and a culture of scientific research to grow. When Silverman became head in 1918 the chemistry faculty were publishing 8-10 journal articles per year and when he retired the faculty were publishing thirty to thirty-five journal articles per year. By the end of Silverman's tenure in 1951, the total number of degrees granted in chemistry by the Department were 394 BSc, 152 MS. and 206 PhD.



Francis Clifford Phillips



Raymond Bacon



Alexander Silvermar



Faculty Highlights: Alexander Star

lexander Star's research group investigates carbon nanomaterials with an emphasis on carbon nanotubes and their potential applications in medicine, defense, energy production, and computation. To advance the field of nanoscience, the Star group explores: (i) the synthesis and characterization of carbon nanomaterials, (ii) the development of nanotechnology enabled chemical sensors and energy conversion devices, and (iii) nanotoxicology and drug delivery.

Synthesis of Novel Carbon-based Nanomaterials via Chemical Vapor Deposition

Employing chemical vapor deposition (CVD), the Star group is developing novel synthetic approaches to carbon-based nanomaterials. For example, they have prepared nitrogen-doped carbon nanotube cups (NCNCs), which appear as stacked cup-like fibers that are $\sim\!\!1~\mu m$ in length and have diameters ranging from 12-40 nm (Fig. 1). Because the graphitic lattice does not grow parallel to the longitudinal axis of the fibers, it is possible to separate long NCNC fibers into short stacked or individual "cups" via mechanical, sonomechanical, and intercalation strategies. These "cups" allow further chemical processing by way of their nitrogen functionalities which are concentrated primarily, though not exclusively, on the open basal plane of the structures.

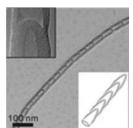


Fig. 1. An SEM image is shown for nitrogen-doped carbon nanotube cups

The Star group is exploring the use of NCNCs as catalysts. Because the NCNCs display catalytic activity for the Oxygen Reduction Reaction (ORR), they are an attractive substitute for noble metals such as Pt or Ru in fuel cell cathodes. Besides low fabrication costs, NCNCs demonstrate resistance to reactive gases

(i.e. poisoning), which is a major advantage over Pt. Further catalytic applications of NCNCs for energy conversion and electrochemical sensing are currently being explored by the Star group.

NCNCs also hold promise as nano-sized containers. Recently, the Star group showed that the open end of the "cups" could be selectively "corked" *via* the growth of gold nanoparticles utilizing HAuCl₄ and the reducing agent, citrate (Fig. 2). By incubating a desired "cargo" with NCNCs prior to "corking," this nanomaterial may prove useful for encapsulating a 'cargo' within their hollow interior cavities. After "corking," they plan to functionalize the 'cups' by employing the nitrogen groups on their basal plane, and then to explore their use for drug delivery.



Fig. 2. This image depicts the separation and corking of NCNCs with gold nanoparticles.

Carbon Nanotube Enabled Sensing

Single-walled carbon nanotubes (SWCNTs), which are composed of a single cylindrical layer of carbon atoms, are prominent in sensor applications because their electrical conductivity is highly sensitive to chemical and biological species. As quasi one-dimensional structures, electrons are confined to the exterior of SWCNTs making them extremely sensitive to perturbations in the local charge environment.

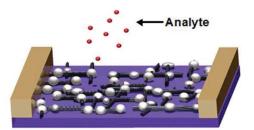


Fig. 3. This schematic shows a single-walled carbon nanotube (SWCNT)-based device that is decorated with a recognition layer (silver regions) sensitive to a particular analyte.

By exploiting the unique electronic properties of SW-CNTs in a field-effect transistor (FET) setup and rendering this nanomaterial selective for an analyte through functionalization with metal nanoparticles, polymers, or biomolecules (Fig. 3), the Star group has developed a range of new chemical and biological sensors. Recently, they demonstrated that SWNT-TiO₂ core/shell hybrid nanostructures exhibit unique electrical behavior in response to UV illumination and acetone vapors. Because acetone is a biomarker for diabetes in the exhaled breath of humans, this novel material may find an important medical use. Also, the Star

group is employing SWCNT-based FETs to study the interactions of lectin-carbohydrates, which have implications for cell-cell recognition, cell-matrix interactions, and viral and bacterial infections.



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University of Pittsburgh

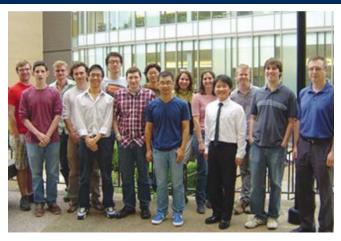


Fig. 4. Star Group, Summer 2013.

Nanotoxicology

As with any new technology, it is important to weigh the benefits of the new materials against their potential hazards. While an ongoing debate exists over the toxicity of CNTs, the Star group (see Fig. 4) is actively quantifying the toxicity and physiological effects of carbon nanomaterials. In collaboration with others, they have demonstrated that carbon nanomaterials undergo enzyme-catalyzed degradation with different peroxidase systems. Their work will have broad implications for carbon nanomaterials including their mass production for utilization in applications.

Faculty Nuggets

Lillian Chong, along with Carlos Camacho, was awarded an NSF MRI grant. The grant represents a joint effort between the Center for Simulation and Modeling (SaM) and the Department of Computational and Systems Biology.

Dennis Curran was awarded the 2014 Ernest Guenther Award in the Chemistry of Natural Products for his creative syntheses of natural products and natural product stereoisomer libraries.

Alex Deiters was awarded a National Science Foundation Division of Molecular and Cellular Biosciences grant to support research aimed at using light to achieve spatial and temporal specificity in the activation of kinases in cells.

Seth Horne received a five-year NIH R01 award based on his proposal, "Molecular Mimics of Protein Tertiary Folding from Primary Sequence Information."

Geoff Hutchison was awarded the Chemical Science Best Poster Prize at the Gordon Research Conference. He was also honored as the Class of 1960 Scholar Lecturer from Williams College.

Kenneth Jordan was the Highlight Lecturer at the Thomas Young Center, University of London.

Kaz Koide's collaboration with Merck was cited in "Marketplace eNewsletter," as demonstrating a rapid method for the evaluation of residual palladium.

Daniel Lambrecht was chosen to be a participant in the CSC New Faculty Workshop in Washington, DC.

Haitao Liu was awarded an Air Force Office of Scientific Research (AFOSR) grant through its Young Investigator Research Program. He also received the Young Investigators Award from the European Materials Research Society.

Xinyu Liu was awarded a Samuel and Emma Winters Foundation Biomedical Research Award, and a career development award from the Melanoma & Skin Cancer Specialized Program of Research Excellence (SPORE) for his research.

Adrian Michael has been appointed president of the Society for Electroanalytical Chemistry (SEAC) for the term 2013-2015.

Jill Millstone received an NSF CAREER Award for her work on 'Surface Chemistry-Controlled Formation of Colloidal Nanoparticle Alloys'.

Renã Robinson received a Keystone Conference Symposium Early Career Travel Award (Keystone Conference on Aging and Diseases of Aging).

Alexander Star received the University of Pittsburgh Innovator Award for his work on a sensor technology.

Michelle Ward, serving as chair, led the Pittsburgh Section of the American Chemical Society in receiving the ACS ChemLuminary Award. Also, Michelle received the 2013 Student Choice Award.

David Waldeck is the 2013 winner of the ACS Pittsburgh Award.

Peter Wipf was awarded the 2013 Edward W. Morley Medal.



University of Pittsburgh

Department of Chemistry

Graduate Awards

Mellon Predoctoral Fellowship Laura Kocsis Youwei Xie

Dietrich School of Arts and Sciences Fellowship

Scott Caplan Scott Crawford Michael Frasso Stephen Groskreutz Michael Hartmann Clinton Johnson Tianyi Luo John Milligan Nicholas Reed Muhammad Salim Erin Shields Odbadrakh Tuguldur Erika Varner Bei Wang William Weller Keith Werling

Goldblatt Fellowship George Lengyel

Bayer Material Science Fellowship Hyo Seong Kim

DeWitt C. Clapp Fellowship Vamsee Voora

Graduate Excellence Fellowship

Chong Liu Zachary Reinert Sarah Wells Daniel Kwak

RKM Graduate Fellowship -Center for Energy Brian Bloom

NSF Graduate Research Fellowship
Stephen Groskreutz



Graduate Highlights:



Tiyeon (Jay) Kim completed her PhD in 2012, under the direction of Professor Shigeru Amemiya. She is currently working as a postdoctoral associate in Professor Allen J. Bard's labs at the University of Texas, Austin, where her research focus is the development of nanoscale scanning electrochemical microscopy (SECM) applications. Her PhD studies strongly support her investigations as a postdoc, which are to improve the spatial resolution of SECM at the nanometer scale.

Jay is also working on a biomedical application that aims to use SECM to detect microbial metabolites. The concept of bacteria in multiple metabolic subpopulations collaborating to promote a locus of infection is a general rule for extracellular pathogens. She is developing SECM as a tool to chemically identify the metabolites that support this replication niche. In addition, SECM

offers the selective probing of replication sites of differing microcolony size as a determinant of growth. By directly monitoring the metabolites in real time and with high spatial resolution, the microbes group behavior can be identified, which can in turn serve as a therapeutic target.

Jiyeon received her BS in chemistry and her MS in analytical chemistry/electrochemistry at Ewha Woman's University. Her research experience includes Ewha Woman's University, Korea Institute of Science and Technology, University of Tennessee, University of Pittsburgh, and University of Texas. Jiyeon has co-authored fifteen publications and she has presented at PITTCON, the ACS, and the Korea Chemistry Society Meetings.

Interdisciplinary Graduate Programs (Biology and Chemistry):

The Department of Chemistry's strength in the chemical aspects of biology, neurochemistry, and medicine is undergoing strong growth and has attracted a number of outstanding graduate students from other programs. The University, with Carnegie Mellon University (CMU), has a graduate program in molecular biophysics and structural biology. This interdisciplinary program, directed by Dr. James Conway at the University of Pittsburgh's School of Medicine, was established by researchers in existing programs in the School of Medicine, Pitt's Dietrich School of Arts and Sciences, and CMU for the benefit of students who want to study at the edges and boundaries of traditional disciplines. Many students from this highly selective program have found a home in chemistry. Karl DeBiec is studying jointly with Professor Lillian Chong (Chemistry) and Angela Gronenborn in (Structural Biology). Karl is using a combination of NMR spectroscopy and computer simulations to characterize the dynamics of a two-domain protein that is linked to plant infection that results in huge losses of rice crops. Sean Carney, working with Professor Michael Trakselis, is using single molecule biophysics to understand the dynamic interactions of DNA with a variety of hexameric DNA replication helicases during unwinding. Helicases are enzymes that assist in the separation of a DNA duplex into single strands. Professor Sandy Asher has three students working with him on various aspects of the improvement and application of UV resonance Raman spectroscopy for determining peptide structure. Elizabeth Dahlburg, David Punihaole, and Jonathan Wert are using this technique to give the first definitive insight into the structure and conformation of fibrils-small fiber-like structures that form in the brains of Huntington's patients. Elucidating the fibril structure will immediately lead to insights into the fibril aggregation mechanism which can in turn be the basis for drug development.

The School of Medicine's Medical Scientist Training Program (aka MD/PhD) is home to a small number of highly talented and focused students. The dozen or so students who arrive each year find a research home in one of a large number of departments at Pitt and CMU. Two recent students in chemistry are Justin Baca (now a resident at Harvard Medical School in emergency medicine) who worked with Professor Asher and Amir Faraji (now a resident at Pitt's medical school in neurosurgery) who worked with Professor Stephen Weber and performed their PhD research in the Department.

Undergraduate In The Spotlight:



his past April the Department celebrated the achievements of our graduating seniors. Over 200 friends and family members joined our graduates and faculty for this happy occasion. Geoff Eddinger is one of those special young people, who received his degree in chemistry. Geoff was very involved in all aspects of our undergraduate program. Geoff carried out research under the direction of Dr. Seth Horne, in which he investigated unnatural backbone oligomers in proteins. He also participated in our Undergraduate Teaching Program as a recitation leader for several organic lectures and as a mentor for an Honors Organic Laboratory class. In addition, Geoff was very active in our American Chemical Society Student Affiliates group and served as a co-outreach coordinator, along with David Palm, for

the past two years. He participated in many of our outreach efforts including the celebration of National Chemistry Week at the Carnegie Science Center and our Saturday Science Programs. Geoff clearly gave of his time to help others achieve as so many of our undergraduates do on a daily basis. Geoff received our Department's Theodore Award which is given to outstanding graduating seniors for overall contributions to our program, and he graduated *summa cum laude*. Geoff is now pursuing graduate studies at the University of Wisconsin. We congratulate Geoff and all of our graduates on a job well done!

UTU Program in General Chemistry

he Chemistry UTU (Undergraduates-Teaching-Undergraduates) project has operated for seventeen years and plays an integral part in the Department's teaching program. Its original goal was to improve students' performance and satisfaction in the general chemistry program, and was funded through the NSF and the Department of Education's FIPSE program. Because of its success, it has spread to other courses (including Organic Chemistry, and the Analytical Chemistry, Instrumental, and Physical Chem-



istry labs), and it displays a diversity in the undergraduate teacher-mentors roles, specific to each course.



In General Chemistry, the UTU program follows the well-proven collaborative small-group model, in which a class of 24 students is organized into 4 groups, each assisted by a UTU. Currently, about 40 UTUs lead groups in recitation and about 30 teach lab each term. The students enjoy and thrive in the discussion-intensive peer-mentored learning environment. The UTU program complements the traditional graduate-TA led recitations and labs, and both benefit by a continuous exchange of ideas between the two models. The group that benefits the most is

surely that of the UTU mentors, who relearn the chemistry through teaching it and improve their communication and organizational skills. They also continue the research tradition by testing new approaches, providing feedback, and thereby enriching the entire General Chemistry teaching program. Several UTUs continue to teach after graduation, and a few go on to seek teacher certification in the School of Education.

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2013 Undergraduate Awards

The American Institute of Chemists Award Matthew A. Baker

The Mary Louise
Theodore Prize
Haddon A. Dine
Geoffrey A. Eddinger
Bradley B. Gilbert
Alexandre Ilitchev
Christine P. Lampe
Akira S. Shimizu
Daniel W. Siroky

The Merck Award
Alexander J. Krisko
Tyler J. Sevco

The SACP College Award
Jonathan C. Weisberg

The Silverman Prize Amanda R. Skopkowski

The Phillips Medal
Jonathon S. Bechtel

The McKeever Summer Undergraduate Research Fellowship Kelsey J. Wiggins

The Wass Summer
Undergraduate Research
Fellowship
Heather A. Fuhrman
Michael S. Mizrahi



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Department Milestones: New Faculty

Alexander Deiters , Professor

Alex Deiters comes to us as a full professor and directs a research program at the interface of synthetic chemistry and biology. His research interests are in the area of synthetic chemistry, synthetic biology, and chemical biology, and range from methodology development for natural product synthesis and the discovery of new therapeutic agents to protein and nucleic acid engineering. Born in Germany, Alex obtained his PhD from the University of Münster in 2000 for work on new cyclization reactions with enantiomerically enriched allyllithium species. He then conducted postdoctoral research at the University of Texas at Austin on the total synthesis of indole alkaloids and later at The Scripps Research Institute on the engineering of new protein function through the incorporation of unnatural amino acids. Alex joined the Department of Chemistry at North Carolina State University as an assistant professor in 2004, were proposed to associate professor in 2004, and to full professor in 2004.



in 2004, was promoted to associate professor in 2009, and to full professor in 2012.

Alex has published over 90 papers and has received several awards for his research, including a Basil O'Connor Starter Scholar Award, a Sigma Xi Research Faculty Award, a Cottrell Scholar Award, a Beckman Young Investigator Award, and an NSF CAREER Award, among others.

Kabirul Islam, Assistant Professor

Kabirul Islam comes to us as an assistant professor from Memorial Sloan-Kettering Cancer Center (MSKCC). As a postdoctoral fellow, he developed a chemical proteomics approach to profile protein methylation, in the group of Professor Minkui Luo. His work has demonstrated that post-translational methylation is not unique to histones; rather a plethora of non-histone proteins can be methylated to regulate diverse biological processes. Kabirul received his PhD for work in natural products synthesis from the Indian Institute of Science, Bangalore; he also did a postdoc at the Rockefeller University where he developed MyoVin-1, a specific small-molecule inhibitor for the motor protein myosin V. Kabirul has 22 journal publications in the fields of total synthesis and chemical biology.



At the University of Pittsburgh Kabirul plans to study the role of epigenetic mechanisms in human health and disease. He will combine his expertise in organic synthesis, mechanistic biochemistry, and proteomics to provide molecular as well as system level understanding of chromatin modifications in gene regulation. Development of small-molecule therapeutics to reverse epigenetic misregulation in human disease will be another major direction in his lab.

Hannah Morris, Lecturer

Hannah Morris comes to us as a lecturer. She earned her PhD from the University of Pittsburgh under the guidance of Patrick Treado and Gilbert Walker. As a postdoctoral fellow at Duquesne, she studied pharmaceutical blending and tablet formulation using near-infrared spectroscopy; she received the Buchi NIR Award in 2001 for that work. From 2000 to 2012, Hannah was the deputy director of the Art Conservation Research Center at Carnegie Mellon University. During her graduate career, Hannah taught general chemistry recitation and laboratory courses. At both Duquesne University and Carnegie Mellon University, she has given guest lectures on general chemistry, spectroscopy, and art conservation topics. In 2012, Hannah became an adjunct faculty member at Rob-



ert Morris University where she taught General Chemistry I and II along with the accompanying laboratory course. This year Hannah is teaching General Chemistry for Engineers I and II.

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New Lab Instructors

Gregg Huston - A former research chemist (DOE, FAA, Pfizer, and Boehringer Ingelheim) and a retired U.S. Army Engineer Officer, Gregg has served as a part time instructor in the Department for a number of years. Gregg also maintains and develops protocols for the gas chromatographs used in the instructional organic laboratories. As a research chemist for DOE's Fossil Fuels Division, he developed methods and instrumentation for trace gas analysis of fluidized bed coal combustion and coal gasification gas streams. For the FAA Gregg managed the development of trace detection systems for explosives, and in the pharmaceutical industry he developed HPLC analysis methods. In the military Gregg managed large scale construction operations in locations throughout the world; he also



managed recovery, clean-up, and structural analysis missions following Hurricane Andrew, the North Ridge earthquake, and Hurricane Katrina. Gregg also ran the Balkans Program for the U.S. Army Corp of Engineers.

Tamika A. Madison - Tamika obtained her PhD from the University of Pittsburgh in 2011. As a graduate researcher, she used computer simulations to study charge transport in organic semiconductors under the direction of Professor Geoffrey Hutchison. She also used a combination of experiment and quantum chemistry calculations to study the Penning ionization of small amides under the direction of the late Professor Peter Siska. As a graduate teaching assistant, she taught recitations and labs in both the general and organic chemistry programs, as well as the Preparation General Chemistry course. Tamika earned the Safford Award for Excellence in Graduate Student Teaching in 2008 and the Safford Fellowship for Excellence in Graduate Student Teaching in 2010. After completing her doctoral work, she taught introductory chemistry at the Community College of Allegheny



County, and general chemistry lectures, recitations, and labs at the University of Pittsburgh.

New Staff Members



Patricia M. Freker: Patty is the payroll/personnel administrator for the Department where she handles the payroll and benefits issues for more than 300 Department personnel. Patty previously worked in the dental school where she processed financial aid in the student services office. She has been with the University for twenty-five years, including nine years at the UPMC Respiratory Care Department.



Christie Hay: Christie is the graduate program administrator where she is responsible for handling all of the administrative needs of the more than 200 graduate students and 30 postdoctoral researchers in the Department. Christie also supports the recruitment and admissions activities for the Department, and she provides support for helping students with job placement. Christie received her graduate and undergraduate degree from Pitt. She is a Navy veteran and a former elementary school teacher in the Pittsburgh Public School District.



Devin Wilcox: Devin is one of the Department's two research stockroom personnel. Devin began to work in the Department of Chemistry as a student worker while finishing his degree in history at the University of Pittsburgh. In addition to working in the Department stockrooms, Devin has worked in the administration and undergraduate studies offices.

Retirements -

Toby M. Chapman, PhD



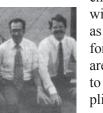
Professor Toby Chapman first came to the University of Pittsburgh in 1967. He started as an assistant professor in the Department of Chemistry, and he was promoted to associate professor in 1974. Toby received his doctorate from the Polytechnic University in New York, where he studied polymer chemistry and anionic styrene copolymerizations. He then became an NSF postdoctoral fellow at Harvard Medical School. Toby has contributed

broadly on the service front in the Department; most recently he served as the assistant chair from

2009 to 2010. Toby has been a mainstay in the Department's sophomore organic chemistry program and its polymer chemistry course for many years. More recently he has contributed to the nursing chemistry and general chemistry programs.

In the early part of Toby's career his research focused on peptide and nucleic acid synthesis; however he soon added more traditional polymer chemistry, including the synthesis of low surface energy polyurethanes and a variety of polymeric amphiphiles of non-traditional structure. His

endeavors soon led to dendritic polymers with mPEG-dend-polylysine copolymers,



(left to right) Professors Stephen Weber, Dennis Curran, Toby Chapman, and Mr. John Enyart

as well as other amine containing polymers based on poly(N-vinyl-formamide). He also studies conjugated dendritic ploymers. These are to be the basis of photochemical hydrogen generation as well as to increase the photoresponse of dye-sensitized solar cells by amplifying the number of dye molecules able to inject electrons. This work has included the synthesis of two generations of a p-(phenylene vinylene) monodendron with porphyrins attached at the termini.

Dr. Chapman is also a member of the American Association for the

Advancement of Science and the American Chemical Society.



Leonard Kogut received his PhD from the University of Pittsburgh in 1970. Len, a senior lecturer in chemistry, retired this past year after seventeen years of service to the Department. Len taught within the general chemistry and engineering chemistry programs, and he served as coordinator of the Freshman Engineering Chemistry Program for many years. In this role he helped to implement the Swanson School's integrated engineering curriculum and the appropriate revision required for our freshman engineering lecture and lab courses. He continued to serve as our liaison with the Swanson School

throughout his tenure. Len was known for his sense of humor, commitment to education, and concern for students' success. We wish him all the best in his retirement.



Dr. Ken Migliorese, PhD, retired in January 2013. He joined the Department in January 2004 as director of technical facilities and instrumentation after a long career as R&D Director at Helene Curtis in Chicago. During his nine years with us, he was involved in all major instrument acquisitions, as well as the design and construction of the building infrastructure needed to support them. Ken was also a key player in both the design and construction of many of the Department's recent renovations, including the renovated

14th and 5th floors in Chevron, renovation of the undergraduate teaching labs on the 2nd, 3rd, and 4th floors of Chevron, replacement/upgrade of the Chevron HVAC system, the Chemistry Instrumentation Center, the Chevron Annex, Chevron/Ashe lobby, Chemistry Library, Coffee Shop, and Computer Classroom, as well as numerous lab and office spaces for both new and existing faculty. Ken's retirement plans include travel and spending time with his grandchildren in Chicago and Washington, D.C.

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Research Support Services and Technical Support

Progress is often measured through change. The Department's facilities have undergone much change over the past few years through updates, renovation, and new construction. Multiple research and teaching laboratories have been modernized; an annex to Chevron was constructed to add synthesis laboratory space; and the Chemistry machine shop and electronics shop have expanded and modernized while merging with those of the Physics and Astronomy Department.

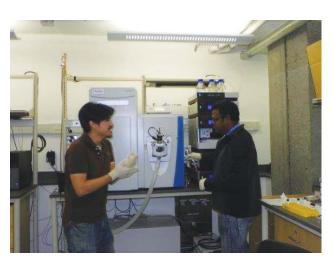
This year is no exception, with the area formerly occupied by our machine shop being modernized to create the Chemistry Instrumentation Center (CIC). The CIC opened in January 2013 and is located adjacent to the fourth floor elevator lobby, at the Chevron end of the tunnel that

leads to Eberly. NMR, Mass Spectrometry, and X-Ray instrumentation are now collected together in a bright and spacious laboratory space that is centrally located for convenient access by all of the Department's research groups. The offices of Dr. Damodaran Achary-Krishnan (NMR), Dr. Bhaskar Godugu (Mass Spectrometry), and Dr. Steven Geib (X-Ray Crystallography) are located within the CIC.



The facility offers state of the art equipment and expertise in support of the Department's research programs. In NMR, the facility has eight high field NMR spectrometers, ranging from 300-700 MHz for solution NMR research and a 500WB for solid state NMR applications. The spectrometers have broad band probes for studies of ¹¹B, ¹⁹F, ²⁷Al, ²⁹Si, ¹¹³Cd, ¹⁹⁵Pt, and ²⁰⁷Pb nuclei, have triple resonance capability for simultaneous pulse on three nuclei, have Pulsed Field Gradient (PFG) capability for 1D and 2D experiments, have automatic shimming and training capabilities, and have auto-samplers.

In Mass Spectrometry, the CIC has three high resolution (HRMS) instruments (Waters Q-Tof, Waters GCT, and Thermo Q-Exactive) and four low resolution (LRMS) instruments (Shimadzu LCMS-2020, Shimadzu GCMS-QP2010S, Shimadzu GCMS-QP5050, and a Voyager MALDI-DE pro). All the LRMS are in an open access area, and are available to trained users 24/7. Samples analyzed in the facility include proteins, peptides, oligonucleotides, oligosaccharides, polymers, and metal complexes as well as other small organic and inorganic molecules.



Recently, advanced proteomics (protein identification) analysis has been implemented in the lab.



University of Pittsburgh



In X-Ray, the CIC has two single crystal diffractometers, a Bruker X8 Prospector Ultra with new copper microfocus source technology and a Bruker Smart Apex with Mo radiation. The new X8 copper microfocus instrument can analyze much smaller crystals than previously possible and it provides new capabilities to determine the absolute structure of light atom organic compounds. It is also configured for biological macromolecules and has proven useful for powder and other non-conventional diffraction experiments.

In addition to the CIC, the Department houses the Materials Characterization Laboratory (MCL), a user facility for materials research that is directed by Dr. Joel Gillespie. The MCL contains more than 50 research instruments that are used for the characterization and analysis of complex materials systems that include polymers, metals and metal alloys, ceramics, semiconductors, and carbon composites. Instruments include advanced atomic force microscopes (AFMs), a Langmuir-Blodgett trough, an Auger electron spectrometer (AES), a contact angle goniometer, and an X-ray photoelectron spectrometer (XPS). The MCL also stewards the Department of Chemistry's shared biological instrumentation cluster and tissue culture laboratory that includes centrifuges, a gel imaging system, autoclaves, incubators, and a fluorescence spectrometer with anisotropy measurement capabilities.

In addition, the facilities for the machine shop and the electronic shop have been renovated and upgraded. The Chemistry and the Physics and Astronomy machine shops have been consolidated into updated space in the former Nuclear Physics Laboratory (NPL) building. Tom Gasmire heads up the new Dietrich School Machine Shop; staff includes Jeff Sicher and newly hired machinists, Josh Byler and Shawn Artman. The Dietrich School Electronics Shop remains on the 3rd floor of Eberly. Electronics specialists include Dave Emala, Chuck Fleishaker, Jim McNerny, Joe Rabel, and George Zuk.







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