

CHEMISTRY

FALL 2014
www.chem.uga.edu

at UGA

Welcome from the Head

Greetings from the Department of Chemistry! This has been another successful year for UGA Chemistry, and I am pleased to report more good news about our department, faculty and students. University enrollment continues to grow each year – this fall, the university enrolled 35,197 students. The increase in student numbers, particularly in the rapidly growing engineering program, has created significant extra demand for Chemistry courses. This growth in instructional demand will help us to make a case for the continued growth of our faculty numbers. As I have mentioned in the past, faculty recruiting is one of the most significant and satisfying parts of my job. In the last year, we were able to recruit a new organic faculty member. Prof. Eric Ferreira comes to us from Colorado State University, where he established a successful and well-funded research program in synthetic organic chemistry. Eric and four of his graduate students moved to Athens over the summer. While his laboratory renovations are taking place, his students are hard at work in temporary space, and his program has hit the ground running. You can read more about Eric and his research activities inside this issue of the newsletter. We have also just completed the recruitment of an organic lecturer, Doug Jackson. Doug is a product of our department, where he is completing his Ph.D. with Richard Morrison. He has had the opportunity to teach courses in the organic program over the last two years, and has established an excellent track record as an instructor. We are fortunate to be able to retain Doug and have high expectations for his contribution to our undergraduate program. In addition, we have two directed faculty recruitment initiatives underway, and I hope to report positive outcomes in the next newsletter.



Jon Amster

Other changes to our faculty have been the retirements of Nigel Adams and Jim Prestegard, which occurred at the end of the spring 2014 semester. Both have been awarded emeritus status, and will continue their research efforts. Nigel Adams moved his research program to UGA from the University of Birmingham (UK) in 1990, and has had a successful and productive program in gas-phase ion chemistry here for the last 24 years. Jim Prestegard moved to UGA from Yale University in 1998, and served as Director of the Complex Carbohydrate Research Center's NMR Facility, and Director of the Resource for Integrated Glycotechnology, a NIH supported research resource. Jim has a primary role in the recruitment of the next NMR Director at the CCRC, and has several active NIH grants that will keep him engaged in research for the foreseeable future. Another change to our faculty took place this summer, when Marcus Lay left UGA to accept a faculty position at Cooper-Union College in New York City. We will miss Marcus and his research program on carbon nanotube sensors.

Our faculty has garnered significant national awards over the last year. Gary Doublerly was the recipient of the Presidential Early Career Award in Science and Engineering. This is the highest honor bestowed by the United States upon outstanding scientists and engineers in the early stages of their career. Gary was presented his award by President Obama in a White House ceremony. We are extremely proud of Gary's success, which has included two other national awards over the last few years, including a NSF Career Award and a DOE Early Career Award. Henry "Fritz" Schaefer won the 2014 ACS Peter Debye Award in Physical Chemistry. The list of previous Debye awardees is a who's-who list of Nobel laureates and National Academy members, standing Fritz in good company. Mike Johnson received a NIH MERIT Award. This award provides 10 years of continuous funding (\$3.3 M) in support of Mike's studies of biological iron-sulfur clusters. Greg Robinson was selected as the UGA recipient of the Southeastern Conference Faculty Achievement Award. Greg has received numerous awards over the last few years, include the ACS Cotton Award in

Construction Begins on Science Learning Center



Rendering of the future Science Learning Center

The long-awaited Science Learning Center (SLC) has finally become a reality, with groundbreaking ceremonies attended by Governor Nathan Deal on August 26. The 122,500-square-foot SLC will house teaching laboratory and lecture facilities for undergraduates in chemistry, biological sciences, plant biology, and physics. It will include 33 instructional lab rooms, two 280-seat tiered lecture halls, two 72-seat scale-up classrooms, lab support areas, and offices for instructional faculty associated with these labs. It will be located at the southwest corner of D. W. Brooks Mall, just south of the College of Pharmacy. Final funding for the project was approved in April, when Gov. Deal signed into law the fiscal year 2015 state budget, which included \$44.7 million for the SLC construction.

When it is completed in 2016, the SLC will relieve a serious space crunch in UGA's south campus science buildings, many built more than half a century ago. For example, the main section of the present Chemistry Building housing undergraduate labs dates to 1960. The impact of the facility will be greatest for the Chemistry Department, which is designated to occupy approximately 60% of the lab space, allowing labs for both General and Organic Chemistry to migrate to the new facility. Once construction of the Science Learning Center concludes, UGA administrators plan to use \$10 million in additional money to modernize the old labs in UGA's Chemistry and Biology buildings. The renovated labs will become expanded facilities for faculty research, hopefully providing space for new faculty.

"This will place the university at the forefront of offering students the very best facilities in science education and will advance the governor's goal of expanding the pipeline for students in the STEM disciplines," UGA president Jere Morehead said in a press release. ●

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Inorganic Chemistry a year ago. Our graduate students have also been the recipients of significant awards. Karson Brooks was awarded a NSF Graduate Fellowship. Karson is a member of Jason Locklin's research group, working in the field of nanoscience and soft polymer materials. Darrah Johnson-McDaniel was awarded a Beverly Hirsh Franklin Graduate Fellowship for Women in Science. Darrah works in the research group of Tina Salguero, and her activities focus on the nanoscience of alkali earth metal silicate materials.

The Science Learning Center, which I mentioned in last year's newsletter, is now under construction. The design phase of this project was completed over the last year, and groundbreaking took place in July. This building will be over 120,000 square feet, and will house teaching laboratories for chemistry, biology, and physics. The construction phase will be completed in the spring of 2016, and we plan to occupy the building for the fall semester of that year. More information and renderings of this building can be found inside this newsletter. Both General Chemistry and Organic Chemistry laboratories will relocate to this building, freeing up close to 20,000 square feet of laboratory space in our present building. We plan to renovate this space and make it available for research, which will allow for the expansion of our faculty numbers and research enterprise.

I hope that you enjoy reading this edition of the Chemistry Newsletter. Our alumni are important to us, and we are happy to communicate our progress and success to you, and to hear of your own, too. Your contributions play an important role in the health of our department, funding seminars, student travel, graduate recruitment, and supporting both our research and instructional missions. I want to take this opportunity to thank you for your generosity, and encourage your continued support of UGA Chemistry. ●



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Paul Schleyer and Tom Zydowsky

2014 Alumni Lecture and Banquet

The Alumni Lecture and Banquet were held on April 18, 2014 in the Chemistry Department and at the Georgia Center for Continuing Education. The lecture in the afternoon was given by **Prof. Paul von Ragué Schleyer** (UGA) on the topic of "The Wonderful World of Carbocations." The highlight in the evening was the presentation of the Distinguished Alumnus Award, which was given to **Dr. Thomas Zydowsky** (Ph.D. 1982, with Prof. Richard Hill).

Paul Schleyer is known internationally for his work in physical organic chemistry, in which he blends synthetic work with computational and spectroscopic studies to elucidate unusual forms of bonding, especially including novel forms of aromaticity. After education at Princeton and Harvard (Ph.D. in physical organic chemistry with P. D. Bartlett) he returned to Princeton and was named Eugene Higgins Professor of Chemistry in 1969. In 1976, he joined the University of Erlangen, Germany, as Co-Director of the Organic Institute and Founding Director of its Computer Chemistry Center (1993). He became Professor Emeritus at Erlangen in 1998, and immediately transitioned to Graham Perdue Professor of Chemistry at Georgia, where he has been ever since.

Schleyer has received many awards and honors and has published widely in areas of organic and inorganic chemistry. He has received honorary doctorates in Lyon, France; Munich, Germany; Kiev, Ukraine; and Marburg, Germany, as well as awards in seven countries and in different areas: physical organic, computational, boron, lithium and most recently theoretical chemistry. He is past President of the World Association of Theoretically-Oriented Chemists (WATOC), a Fellow of the Bavarian Academy and the International Academy of Quantum Molecular Science, as well as the American Academy of Arts and Sciences, Coeditor of the Journal of Computational Chemistry, and was the Editor-in-Chief of the Encyclopedia of Computational Chemistry. His 12 books deal with carbonium ions, *ab initio* molecular orbital theory, and lithium chemistry, as well as *ab initio* structures, and involve collaborations with Leo Radom, as well as with Nobel Laureates H. C. Brown, G. A. Olah, and J. A. Pople. He has published more than 1200 papers. His H-index of 119 is the seventh highest among chemists internationally.

Dr. Tom Zydowsky is senior scientist and the head of pharmaceutical development in the HIV and AIDS Program at the Population Council's

Center for Biomedical Research in New York City. He leads a multidisciplinary team of scientists developing microbicides, which are drug loaded prophylactic products (films, gels, tablets, or vaginal rings) used to prevent the acquisition and transmission of HIV and other sexually transmitted infections (STIs).

Tom was born in Chicago and later moved to Norridge, IL, where he attended public schools. He received his B.S. in Chemistry at Northern Illinois University in 1975 and an M.S. in Organic Chemistry (David M. Piatak) there in 1978. He started at UGA in the fall of 1978, and received his Ph.D. with Dick Hill in June 1982.

Following an NIH postdoc with Heinz Floss and Leo Paquette at Ohio State, Tom joined Abbott Laboratories, designing and synthesizing renin inhibitors, angiotensin II antagonists, and nitric oxide synthase inhibitors. He also worked at Cubist Pharmaceuticals (anti-infectives), Shipley Company (semiconductor materials), Eisai Research Institute (GPCR inhibitors), and FMC Corporation (GABA inhibitors and muscarinic agonists), before joining the Population Council in 2007.

Tom is also a freelance writer, specializing in scientific biographies of influential chemists. His article on R. B. Woodward, entitled *Of Sandwiches and Nobel Prizes*, describes Woodward's reaction to not getting the 1973 Nobel Prize in Chemistry, which was awarded to Fischer and Wilkinson for their contributions to the chemistry of organometallic sandwich compounds. Tom has written other short bios since then, but the ferrocene story is his favorite. The article is available at: tinyurl.com/q8ofedr.



Prof. Alan Marshall

The Alumni Lecture and Banquet will be held next year on Friday April 17, 2015. The speaker will be **Prof. Alan Marshall**, from Florida State University and the National High Magnetic Field Laboratory. ●

New Faculty

Welcome New Faculty: Eric Ferreira

Dr. Eric Ferreira joined the faculty as an Associate Professor in August 2014. Ferreira performed his undergraduate studies at MIT, where he spent some time doing research under the direction of Prof. Stephen Buchwald. From there, he then pursued his graduate degree at Cal Tech with Prof. Brian Stoltz. His research focused on the development of synthetically useful novel oxidation systems using palladium catalysis. Upon completion of his Ph.D., he continued his studies as an American Cancer Society Postdoctoral Fellow at Stanford University with Prof. Barry Trost, where his work concerned the use of ruthenium and palladium catalyzed cycloisomerizations for the formation of polycyclic compounds. He began his independent career as an Assistant Professor in the Chemistry



Associate Prof. Eric Ferreira

Department at Colorado State University in 2008, before moving to UGA in 2014.

Research in the Ferreira group is focused on the design and development of new synthetic transformations, primarily centered around transition metal catalysis. Critical to this effort is the ability to derive inspiration from both reaction mechanisms and natural products. The understanding of intermediates along mechanistic pathways makes it possible to design innovative chemical transformations that can capitalize on these potentially reactive species. Natural products possessing interesting biological activity and structural properties, and our analyses of their respective core molecular architectures, inspires the invention of synthetically relevant methods. Ultimately, explorations in these areas will deepen the understanding of fundamental principles of catalysis and reactivity.

Research is presently focused in several areas. A primary activity is the broad application of catalytic alkyne activation processes in synthetic forays, including the total syntheses of complex molecules featuring promising anticancer, anti-neurodegenerative, and antibacterial properties. A second area of research has been in the invention of molecular scaffolds that induce selective catalytic functionalizations of inherently unreactive bonds. A more recent program has been initiated toward the design of catalytic transformations based on earth-abundant metals, emphasizing the importance of developing sustainable synthetic processes for chemical industry. This research has been supported by the National Institutes of Health, the National Science Foundation, the Environmental Protection Agency, and the American Chemical Society, among others. Ferreira is enthusiastic about developing his new research program at UGA. ●

Fritz Schaefer Receives 2014 Peter Debye Award in Physical Chemistry



Prof. Henry "Fritz" Schaefer, Graham Perdue Professor of Chemistry, received the 2014 Peter Debye Award in Physical Chemistry sponsored by the E. I. du Pont de Nemours & Company. The American Chemical Society announced the 2014 ACS National Awards in the September 9th issue of *Chemical & Engineering News*, and the award was presented at the National ACS Meeting in San Francisco in August.

The award is named for Peter Debye (1884-1966), a Dutch-American physicist, chemist and Nobel laureate who was successor to Albert Einstein in several academic appointments in Europe in the early 20th Century. In 1912, Debye extended Einstein's theory of specific heat and developed a method that became known as the Debye Model for estimating the phonon contribution to the heat capacity in a solid. The Award is one of the most prestigious given by ACS.

Director of the Center for Computational Quantum Chemistry at UGA, Schaefer was recognized for the development of new methods in quantum chemistry, and for many applications to molecular structure, spectroscopy and reaction dynamics.

"I am thankful to receive this recognition. However, the real credit must go to the past and present members of my research group, most of whom have been extraordinary Ph.D. students, gifted postdoctoral fellows and a half dozen amazing senior group members," Schaefer said. "My philosophy is first and foremost to do all I can to develop truly independent young scientists. This means giving them great freedom, including the ability to make plenty of mistakes. The result being a remarkable group of scientists who have done outstanding science with me and gone on to positions of great distinction in academia, at national laboratories, and in industry."

Schaefer has previously been honored with several prestigious awards for his discoveries in chemistry including the Chemical Pioneer Award from the American Institute of Chemists and the Humboldt Research Award from Germany's Alexander von Humboldt Foundation.

"This award confirms what many people already know about Fritz Schaefer. He is a world-renowned computational chemist whose work has impacted every area of chemistry," said Jonathan Amster, professor and head of the Department of Chemistry. "He is a tremendous asset to our department and to the university. ●"

Prof. Michael Johnson Receives NIH Merit Award



Michael K. Johnson, Distinguished Research Professor and Co-Director of the Center for Metalloenzymes Studies, has received a National Institutes of Health MERIT award (\$3.3M over 10 years). The objective of NIH MERIT Awards is to provide long-term, stable support to investigators with "outstanding records of productivity, creativity and impact in biomedical research and outstanding records of service to the scientific community." Dr. Johnson has

had continuous NIH support for the past 29 years and the MERIT award was for his outstanding contributions to understanding the biogenesis and repair of biological iron-sulfur clusters and to promoting interdisciplinary training in bioinorganic chemistry. The medical significance of his research program stems from the fact that numerous important biological processes in humans involve proteins containing iron-sulfur clusters. However, these ancient cofactors are readily degraded by oxygen or reactive oxygen species resulting in loss of protein function. Consequently understanding iron-sulfur cluster assembly and repair are essential for understanding the aging process, age-related neurodegenerative diseases such as Parkinson's and Alzheimer's, and other diseases such as cancer and atherosclerosis, all of which have been associated with oxidative stress. Using biophysical spectroscopic techniques, the Johnson group recently made major progress in unravelling the molecular mechanisms of iron-sulfur cluster assembly, degradation and repair. This extremely prestigious award will enable the Johnson group to continue and expand this pioneering research program. ●

2013 R. B. King Lecture

The 2013 R. B. King Lecture took place on November 5, 2013 in the Chemistry Department, with a reception and dinner that night. The lecture was presented by Prof. Richard Schrock, Frederick G. Keyes Professor of Chemistry at MIT, on the subject of "Olefin Metathesis by Mo and W Catalysts: Not Just Chopped Liver."

Professor Schrock was born on January 4, 1945 in Berne, Indiana. After his family moved to San Diego in 1959, he attended UC-Riverside, graduating with a B.A. in Chemistry in 1967. He went on to graduate school at Harvard, where he worked with Prof. John Osborn, receiving his Ph.D. in 1971. Following a postdoctoral fellowship with Prof. Jack Lewis at Cambridge, Schrock accepted a position at the DuPont Experimental Station in 1972. He joined the faculty at MIT in 1975, where he has been ever since.

Prof. Schrock received the Nobel Prize in Chemistry in 2005 together with Robert H. Grubbs and Yves Chauvin for his work in olefin metathesis. This area of work uses transition metal complexes as catalysts for the processing and synthesis of a variety of organic chemicals, many of which are used in the pharmaceutical industry. ●



Richard Schrock and Bruce King

Professor Gary Douberly Receives Presidential Early Career Award for Scientists and Engineers

Associate Professor **Gary Douberly** recently received one of the highly prestigious Presidential Early Career Award for Scientist and Engineers (PECASE) from the White House Office of Science and Technology Policy. The award was given for "foundational spectroscopic studies of previously unobserved, complex hydrocarbon combustion intermediates critical to the understanding of ignition and soot formation; and for service to undergraduates and the scientific community."

PECASE awards are the highest honor bestowed by the United States Government on science and engineering professionals in the early stages of their independent research careers. The awards, established by President Clinton in 1996, are coordinated by the Office of Science and Technology Policy within the Executive Office of the President. Awardees are selected for their pursuit of innovative research at the frontiers of science and technology and their commitment to community service as demonstrated through scientific leadership, public education, or community outreach. The winners received their awards at a Washington, DC, ceremony on the 14th of April, 2014 attended by President Obama.

"The impressive achievements of these early-stage scientists and engineers are promising indicators of even greater successes ahead," Obama said. "We are grateful for their commitment to generating the scientific and technical advancements that will ensure America's global leadership for many years to come."

Federal science agencies join together annually

to nominate the most meritorious scientists and engineers whose early accomplishments show the greatest promise for assuring America's preeminence in science and engineering and contributing to the awarding agencies' missions. Douberly was nominated by the Chemical Physics Program of the Chemical Sciences, Geosciences, & Biosciences Division, Office of Science, of the U. S. Department of Energy for his work on the isolation and stabilization of transient combustion intermediates in ultra-low temperature superfluid helium droplets. Professor Douberly has made significant contributions to the development of helium nanodroplet isolation spectroscopy, a novel technique where droplets of liquid helium freeze out high energy metastable configurations of a reacting system, permitting laser spectroscopic characterizations of products and intermediates that result from hydrocarbon radical reactions with molecular oxygen and other small molecules relevant to combustion environments. The majority of these transient species have never been directly observed in traditional spectroscopy experiments. Professor Douberly's research group is developing methods to carry out the first direct observation of the elusive hydroperoxyalkyl radicals (QOOH) and their oxygen adducts (O_2QOOH), which are important in the low temperature hydrocarbon oxidation chemistry associated with homogeneous charge compression



Dr. Patricia Dehmer, Department of Energy, Office of Science Deputy Director for Science Programs and Dr. Ernest Moniz, U.S. Secretary of Energy

ignition (HCCI) engines. These studies aim to improve our understanding of the detailed mechanisms of hydrocarbon combustion, resulting in more accurate predictive combustion models.

Douberly received a B.S. degree in Chemistry from the University of Central Florida in 2000 and a Ph.D. in Physical Chemistry from the University of North Carolina at Chapel Hill in 2006 under the direction of Roger E. Miller and Tomas Baer. Following postdoctoral work with Michael A. Duncan at the University of Georgia, he began his faculty appointment at UGA in 2008. In addition to the PECASE award, Professor Douberly has received the Early Career Research Program Award from the DOE Office of Science, the CAREER award from the National Science Foundation, the Rao Prize, and the *Journal of Physical Chemistry A* Lectureship Award. ●



Gregory H. Robinson Receives SEC Faculty Achievement Award

Gregory H. Robinson, Foundation Distinguished Professor of Chemistry, has been named the University of Georgia's 2014 recipient of the Southeastern Conference Faculty Achievement Award.

The award, which is administered by SEC provosts, recognizes one faculty member from each of the 14 SEC schools and includes a \$5,000 honorarium. It honors professors with outstanding records in

teaching and scholarship who serve as role models for other faculty and students. Robinson received his undergraduate degree in chemistry from Jacksonville State University and earned his doctorate in chemistry from the University of Alabama. He served on the faculty at Clemson University before joining the UGA faculty in 1995. He was named Distinguished Research Professor in 2000, Franklin Professor in 2005, and Foundation Distinguished Professor in 2013.

"Dr. Robinson excels as a scholar and as an instructor who demonstrates an outstanding level of commitment to the university and to his field," said Pamela Whitten, Senior Vice President for Academic Affairs and Provost. "He represents the University of Georgia with distinction in all that he does and is most deserving of this honor."

Over the past 25 years, Robinson and his team have published a series of fundamental findings that have reshaped how scientists view chemical bonding in many inorganic compounds. His achievements have been described as groundbreaking, and his work is internationally recognized. Robinson has presented his research in nearly 150 peer-reviewed journal articles, six book chapters, a book, and dozens of regional, national and international conference presentations.

The Franklin College of Arts and Sciences professor has received a number

of honors, including the Humboldt Research Award granted by Germany's Alexander von Humboldt Foundation. The award is granted in recognition of a researcher's career achievements and is granted to those academics whose fundamental discoveries, new theories or insights have significantly impacted their own discipline. Robinson also recently received the F. Albert Cotton Award in Synthetic Inorganic Chemistry, sponsored by the American Chemical Society, which recognizes distinguished work in synthetic inorganic chemistry. His additional awards include the National Science Foundation's Award for Special Creativity, the Percy L. Julian Award of the National Organization of Black Chemists and Chemical Engineers, and the University's Lamar Dodd Research Award.

Robinson teaches a range of courses in chemistry, including large introductory chemistry classes, upper-division inorganic chemistry courses and graduate-level seminars. Student evaluations speak of his "great personality," his "great sense of humor," and his "ability to break concepts up into their most basic parts to allow for complete conceptual understanding." Robinson also has taught several First-Year Odyssey Seminars and he has supervised nearly three dozen undergraduates conducting research in his lab. He has served as major professor for 15 doctoral-level students and sponsored a number of post-doctoral fellows in his lab.

Despite his research and teaching commitments, Robinson is active in service to his university and to his profession. On campus, he mentors student-athletes and serves on the UGA Research Foundation as well as on the UGA Athletic Association Board of Directors. He has been a consultant or panelist for the National Science Foundation and the Ford Foundation and sits on the editorial boards of seven journals in his field. Robinson also visits elementary schools to talk with children about chemistry and what it means to be a chemist. ●

Chemistry Graduate Student Awarded NSF Graduate Fellowship



Karson Brooks, second year graduate student working under the direction of Professor Jason Locklin, has won an NSF Graduate Research Fellowship for her work in “macromolecular, supramolecular, and nanochemistry.” Karson was one of only eleven UGA students to win an NSF fellowship this year, and the only graduate student in the Chemistry Department to do so. She is the first chemistry graduate student to win the award in many years.

Karson graduated from the University of Alabama, Tuscaloosa, where she accrued numerous academic accolades, was a member of several honor societies, and made the President’s List for eight consecutive semesters. In addition to extensive undergraduate research, she also served as a 3M Research Fellow at Pennsylvania State University.

NSF Graduate Fellowships are among the most competitive available to graduate students in the sciences, and are often awarded to individuals who go on to “become life-long leaders that contribute significantly to both scientific innovation and teaching.” Previous winners include former U.S. Secretary of Energy Stephen Chu, Google Founder Sergey Brin, and numerous Nobel Prize laureates. The award provides three years of financial support, including a stipend and education allowance, as well as professional development and international research opportunities. Only 2,000 fellowships were awarded nationally from a pool of 14,000 applicants.

UGA Chemistry Ph.D. Graduate Awarded Merck Fellowship



Robert J. Gilliard, Jr., a 2014 doctoral graduate in the University of Georgia Franklin College of Arts and Sciences Department of Chemistry, has been awarded a UNCF/Merck Foundation Postdoctoral Science Research Fellowship. The Awards are a component of the UNCF/Merck Science Initiative to support the training and development of world-class African American biomedical research scientists. The award

provides \$98,000 and includes a stipend, research grant, and travel funds for up to two years of fellowship tenure.

Gilliard will pursue research projects focused on synthetic chemistry, collaborating with John Protasiewicz at Case Western Reserve University in Cleveland, OH and Hansjörg Grützmacher at ETH Zürich, an engineering, science, technology, mathematics and management university in Zürich, Switzerland. Gilliard left for Zürich in August.

“This is a tremendous honor for which I am extremely grateful,” said Gilliard, a native of Hartsville, SC, who came to UGA in 2009 to work with Prof. Gregory H. Robinson. “My experience at UGA has been highly rewarding, in research as well as teaching, and I’m looking forward to these new opportunities for collaboration.”

Gilliard’s research at UGA has focused on the chemistry of

beryllium, a highly toxic element that has historically presented a number of experimental challenges. After working with Professor Rhett C. Smith and graduating from Clemson University, he decided to continue in organometallic chemistry. “I searched all the programs and people in the Southeast to find the best faculty member to work with, and came to UGA to work with Greg Robinson.”

Awarded the Outstanding Teaching Award and the K. W. Whitten Award in the Department of Chemistry in 2010, Gilliard received the Outstanding Teaching Award from the UGA Graduate School in 2011 and 2012. In 2013, he received the Martin Reynolds Smith Prize for best chemical research publication and he was one of a select group of young American scientists chosen to attend the 63rd Lindau Nobel Laureate Meeting, a global forum “to educate, inspire and connect the world’s international best talents.”

“The Merck Postdoctoral Fellowship is a prestigious honor, not just for Robert but also for the Department of Chemistry and the University of Georgia,” said Robinson, Gilliard’s mentor and advisor. “Robert arrived at UGA with a clear career plan and he has worked hard to realize his ambition, forging new directions in the synthetic organic chemistry of beryllium.”

“One cannot practice chemistry alone and the team here at UGA, from the very sharp undergraduates working in our labs to our great faculty, everyone has been instrumental in my success,” Gilliard said. “Greg Robinson, Fritz Schaefer and Paul Schleyer are among the top chemists in the world, right here on campus, and it has been an incredible honor learning from the best.”

Chemistry Student Honored with Beverly Hirsh Frank Graduate Fellowship



For the second year in a row, UGA’s Graduate School has honored an outstanding doctoral student in the Department of Chemistry with a Beverly Hirsh Frank Graduate Fellowship for Women in Science. **Darrah Johnson-McDaniel** is the 2014 recipient of this award, which provides special recognition of her original research in an interdisciplinary and emerging field.

Darrah is beginning her 4th year of study with Prof. Tina Salguero. Her research has pioneered the nanoscience of alkali earth metal silicate materials, some of which have a long history dating back to ancient Egypt and Mesopotamia. According to Prof. Salguero’s nomination, “Darrah has reinvented this ancient material for the modern world with state-of-the-art chemistry and materials science techniques.” To date Darrah has published three manuscripts on this topic, notably a widely publicized 2013 article in the *Journal of the American Chemical Society* (“Nanoscience of an Ancient Pigment”).

In addition to these research achievements, Darrah received a 2014 Graduate Teaching Assistant Award and the 2014 Kenneth W. Whitten Award for her contributions to upper level undergraduate chemistry courses and participation in Franklin College’s Writing Intensive Program.

Darrah received her B.S. in Chemistry degree from UGA in 2010. After graduation she plans on a career in government or industry R&D.

Beverly Hirsh Frank (A.B., ‘54) is the generous benefactor of this fellowship and other activities at her alma mater. ●



Ken Whitten (left) and Richard Morrison (right), with (from left to right) Kenneth Whitten Award winners David McDonald, Kasey Darley and Darrah Johnson-McDaniel.

Northeast Georgia ACS Spring Awards

The N.E. Georgia Section of the ACS held its annual awards banquet on April 18 at the Georgia Center. This year's banquet was combined with the Alumni Appreciation Banquet. Several of our professors and students were honored with awards from the local section this year. Dr. Richard Hubbard received the George Philbrook Award for Outstanding Undergraduate Teaching, while Prof. Gary Douberly was recognized as the Chemist of the Year for Research. Doug Jackson was recognized as the Outstanding Graduate Student of the Year, while Outstanding Undergraduate Students of the Year awards were given to Philip Grayeski and Zachary Husk.

In addition to the local ACS awards, Chemistry Department Award winners were also recognized. These included Michael Dibble (Pamela Ann Henkel Award for most outstanding undergraduate in Organic Chemistry), Nichole Schwartz (Alfred W. Scott Award for most outstanding rising senior), Trenton Berding (L. B. "Buck" Rogers Award for outstanding research by an undergraduate student), and Alexander Sokolov (Martin Reynolds Smith Award for best research paper by a graduate student). David McDonald, Darrah Johnson-McDaniel and Kasey Darley all won Kenneth Whitten Awards for Outstanding Teaching Assistants. ●

Outstanding TAs for 2014

The UGA Center for Teaching and Learning, the Office of the Senior Vice President for Academic Affairs and Provost and the UGA Graduate School has announced the recipients of the 2014 Outstanding Teaching Assistant Awards, a UGA campus-wide honor. Seven graduate students in the Department of Chemistry were selected as recipients of this distinction. These graduate students, Darya Asheghali, Nidhi Bhatt, Darrah Johnson-McDaniel, Molly Larkins, Brandon Magers, Charles Stanton and Ramsey Steiner, are recognized for their strong abilities and high standards as teaching assistants and their commitment to excellence.

Darya Asheghali, Nidhi Bhatt, Molly Larkins and Brandon Magers were nominated for their efforts in undergraduate general chemistry laboratories. Charles Stanton and Ramsey Steiner were nominated for their efforts in undergraduate organic chemistry laboratories. Darrah Johnson McDaniel was nominated for her efforts in general chemistry, in an inorganic special topics course, and in an advanced chemistry laboratory course.

The UGA Center for Teaching and Learning annually recognizes the efforts of teaching assistants towards maintaining excellence in classroom and laboratory instruction at UGA. The Outstanding Teaching Award is conferred on those teaching assistants, nominated



From Left to Right: Ramsey Steiner, Molly Larkins, Darrah Johnson-McDaniel, Nidhi Bhatt, Darya Asheghali, Charles Stanton, and Brandon Magers

by their departments, who personify the very best in undergraduate instruction, and go well above and beyond what is required to enhance the learning experience for their students. ●

Spring Reception Honors 2014 Chemistry Graduates



First row left to right: Holly Hodges, Malikhah Christie, Caitlin Ruddick, Meredith Martin, Shannon Rivera, and Elizabeth Heying. Second row left to right: Robert French, Ashley Althoff, Mary Baggett, Michael Dibble, Meredith Beck, Travis Welsh, Wenbo Xie, Erik Bodel, Tristin Thompson, Kimberly Yau, and Martha McGill. Third row from left to right: Philip Grayeski, Mark Sims, Orrett Walker, Ian Webster, Timothy Watson, Anthony Hamilton, Tyler Huseman, Isaiah Norris, Brian Croft, and Zachary Fultz

41 seniors graduated with degrees in Chemistry at the end of spring semester 2014. The Chemistry Department honored these graduating seniors with a reception on graduation day last May in the Miller Learning Center Rotunda. Faculty, staff, seniors and their families attended. Undergrad Advisor Prof. Gary Douberly recognized each of the seniors present, noting their various activities and accomplishments throughout their undergraduate careers, including the impressive statistic that 14 of these seniors graduated with GPAs greater than 3.5. He also outlined the future employment or educational plans for each student. All were encouraged to return to UGA often for visits and to send money to Chemistry regularly! ●

2014 Philbrook Scholars

Three students in the incoming graduate class for the 2014-2015 academic year, **Benjamin Cline**, **Marissa Estep**, and **Peter Franke**, have been designated Philbrook Scholars. The Philbrook Scholarship “recognizes academic and research excellence in chemistry at the undergraduate level, and the potential for outstanding contributions at the graduate level and beyond.”

The Philbrook Scholarship program was established in 2010 with a generous gift from alumnus Dr. Ernest Drew. Dr. Drew earned his B.S. degree in Chemistry from UGA in 1958, and he went on to earn his Ph.D. in Chemistry from the University of Illinois in 1962. The program is named for George E. Philbrook, Professor of Chemistry at UGA from 1946 to 1974. Since 2010, with continuing support from Dr. Drew, seventeen graduate students have been recognized as Philbrook Scholars and have received support through the program.

Benjamin Cline earned his B.S. degree in Food Science from Cornell University, along the way also earning many prestigious scholarships and awards. He has a strong and varied research background in both academic and industrial research and development. Applying his interest in chemistry to food science, he's developed ice cream flavors, devised strategies to reduce suspended solids in waste water, evaluated nutritional value of sports drinks, assessed microbial compositions of foods, in addition to numerous other research projects he's pursued in the food sciences. As a senior, he developed an interest in nanoscale analytical techniques, and discovered the ongoing research in Prof. Richard Dluhy's lab at UGA. Benjamin began conducting research with Dr. Dluhy in January of 2014 and will continue with Dr. Dluhy for his doctoral research.

Marissa Estep earned B.S. degrees in both Mathematics and Biochemistry and Molecular Biology, with a minor in Chemistry, from Liberty University in Virginia. Included among her many honors and awards is a National Merit Finalist scholarship. She has a strong research background, which began with both experimental and theoretical organic chemistry at Liberty where she worked with Prof. Michael Korn. Having developed an interest in theoretical and computational chemistry, she earned a spot in the Summer



Benjamin Cline, Marissa Estep, and Peter Franke

Undergraduate Research Fellowship Program at the Center for Computational Quantum Chemistry at UGA, working with Prof. Fritz Schaefer, and earned authorship on a manuscript as a result of her research efforts. More recently, she performed research in biological and bioinorganic chemistry both at Liberty and at Virginia Tech with Prof. Dennis Dean as part of a NSF REU program. Marissa matriculated early as part of the UGA Summer Bridge program and is currently performing research once again with Prof. Schaefer.

Peter Franke earned his B.S. degree in Chemistry, with a minor in mathematics, from Virginia Commonwealth University. He's received many academic awards and honors including the prestigious VCU Provost Scholarship. His research interests are in the areas of physical and computational chemistry, materials science, spectroscopy and mathematics. With Prof. Samy El-Shall at VCU, he synthesized various nanocomposite materials and characterized them spectroscopically in order to test hypotheses concerning the intermolecular forces maintaining the structures of the materials. He also conducted innovative research to simultaneously polymerize and laser-reduce graphene oxide to graphene. He has joined the group of Prof. Gary Douberly to pursue research that emphasizes both experimental spectroscopy and theory/computation. ●

Hines and Grimes Distinguished Fellowships to Chemistry Graduate Students



From Left to Right: Brian Sanders, Sean Marrache, and Anthony Prudden

Three graduate students in the Department of Chemistry recently earned distinction from the Franklin College of Arts and Sciences at the University of Georgia as recipients of distinguished fellowships. Brian Sanders is the 2014 recipient of the prestigious Mary Laraine Young Hines Graduate Fellowship in Cancer Research, while Sean Marrache and Anthony Prudden are the 2014 recipients of prestigious Grimes Family Distinguished Graduate Fellowships in Natural Sciences. These fellowships support excellence, innovation, dedication and creativity in graduate

research related to cancer.

Brian Sanders is a doctoral student under the direction of Prof. Todd Harrop, and is the sole recipient of the Hines Fellowship this year. Brian's research in bioinorganic chemistry focuses on synthesizing and characterizing heme-like molecules for effecting transformations between nitrogen oxide species, which has important implications in many areas including bioremediation, cardiovascular disease and cancer.

Sean Marrache recently graduated with his Ph.D., working with Prof. Shanta Dhar. Sean's research was on the development of organelle-targeted nanocarriers for the treatment of a variety of different cancers, which could improve upon current chemo-therapeutics in the clinic today.

Anthony Prudden is also the recipient of the 2013 Grimes award. Anthony is a doctoral student working under the direction of Prof. Geert-Jan Boons. Anthony is developing novel methods for synthesis of oligosaccharides found on cancer cells, which is key for understanding the roles of these carbohydrate molecules in cancer.

Mary Laraine Young Hines graduated from UGA in 1968 with a degree in English. She subsequently earned degrees from both UNC-Chapel Hill and Duke. Her career includes work with the American Red Cross, the USO, Duke University Admissions, the Raleigh Fine Arts Society, the Daughters of the American Revolution, as well as work as a special educator and realtor. Mrs. Patricia R. Grimes graduated from UGA in 1970 with a degree in mathematics and subsequently had a successful career in technology and banking, and was named Senior Vice President for Sun Trust supervising all application programming for the more than 50 Sun Trust locations. ●

News

New Aspirin-Based Prodrug May Prevent Damage Caused by Chemotherapy

Researchers at the University of Georgia have developed a new prodrug that promises to reduce many of the negative side effects caused by cisplatin, a commonly prescribed chemotherapy treatment.

Cisplatin may be used to treat a variety of cancers, but it is most commonly prescribed for cancer of the bladder, ovaries, cervix, testicles and lung. It is an effective drug, but it often causes severe and irreversible damage to a patient's kidneys, hearing and sense of balance.

UGA researchers combined cisplatin with aspirin in a new single prodrug formulation they call Platin-A, which prevents these negative side effects by reducing inflammation. They reported their findings recently in *Angewandte Chemie*, a journal published by the German Chemical Society.

"We know that inflammation plays a major role in the development of these side effects," said Rakesh Pathak, lead author of the paper and postdoctoral research associate in the UGA Chemistry Department. "By attaching aspirin to cisplatin, we can help control this response and reduce damage to the body."

Reducing these negative side effects will not only provide the patient with a better quality of life during and after treatment, but it may also make oncologists less hesitant to prescribe cisplatin.

Prodrugs like Platin-A enter the body in a mostly inactive state, but they are converted to their active state after going through normal metabolic processes. Prodrugs allow scientists to have more control over



the simultaneous release of both drugs and how long it remains active.

"You could administer aspirin separately from chemotherapy, but it would not be as effective as this prodrug formulation," said Shanta Dhar, Assistant Professor of Chemistry and principal investigator for the project. "It's a bit like making a cocktail," she said. "You could drink each of the ingredients one by one, but it works much better if you put it all in the same glass first."

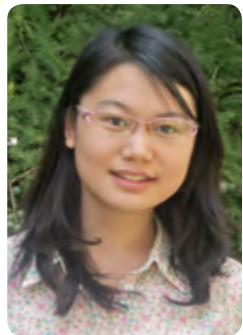
Both Dhar and Pathak caution that their experimental results are preliminary and they must do more work before this is tested in living organisms. However, they say the new formulation shows great promise. While this project focused specifically on prostate cancer and one chemotherapy drug as a model, they believe that the same approach could work for many other forms of cancer and their preferred treatment.

"We are now developing a platform where we can plug in any chemotherapy with any anti-inflammatory and find out which combinations work best," Dhar said.

The researchers also plan to incorporate this technology into their ongoing work with nanotherapeutics. Dhar's NanoTherapeutics Research lab has created numerous nanoparticles, each one 1,000 times finer than the width of a human hair, which they use to attack pathogens and deliver drugs.

"If we use nanoparticles to deliver our prodrug, we can control where it goes and how it breaks down with even more precision," said Dhar, who is also a member of UGA's Cancer Center, Nanoscale Science and Engineering Center, and Center for Drug Discovery. "This is our next step." ●

UGA Researchers Developed a Novel Nanoparticle for Magnetic Resonance Imaging



Wei Tang

graduate student **Wei Tang**, and her advisor **Dr. Jin Xie**, along with their collaborators.

The team used a high temperature decomposition method to prepare the Fe_5C_2 nanoparticles. The as-prepared products are coated with hydrophobic alkyls and cannot be dispersed in water. For uses in bio-related applications, the researchers added a second, phospholipid coating onto the particle surface to render them water soluble. The resulting nanomaterials possess strong and stable magnetization in the air. Also, they showed low toxicity in cell

Iron Carbide, Fe_5C_2 , has long been used in metallic alloys and hard coatings for its superior resilience. Less known is that this compound also displays strong magnetism and good biocompatibility, making it a promising biomaterial with applications in fields like magnetic resonance imaging (MRI) and magnetic separation. However, these applications require Fe_5C_2 to be made in the form of colloidally stable nanoparticles, which has proven to be challenging. This problem was solved recently by UGA

toxicity studies. More impressively, the particles exhibit an r_2 relaxivity — which is a measure of a material's ability to induce contrast in MRI — of $464.02 \text{ mM}^{-1}\text{s}^{-1}$. This value is among the highest of all the MRI contrast probes reported so far. As a comparison, clinically used Fe_3O_4 nanoparticles have an r_2 of $\sim 100 \text{ mM}^{-1}\text{s}^{-1}$.

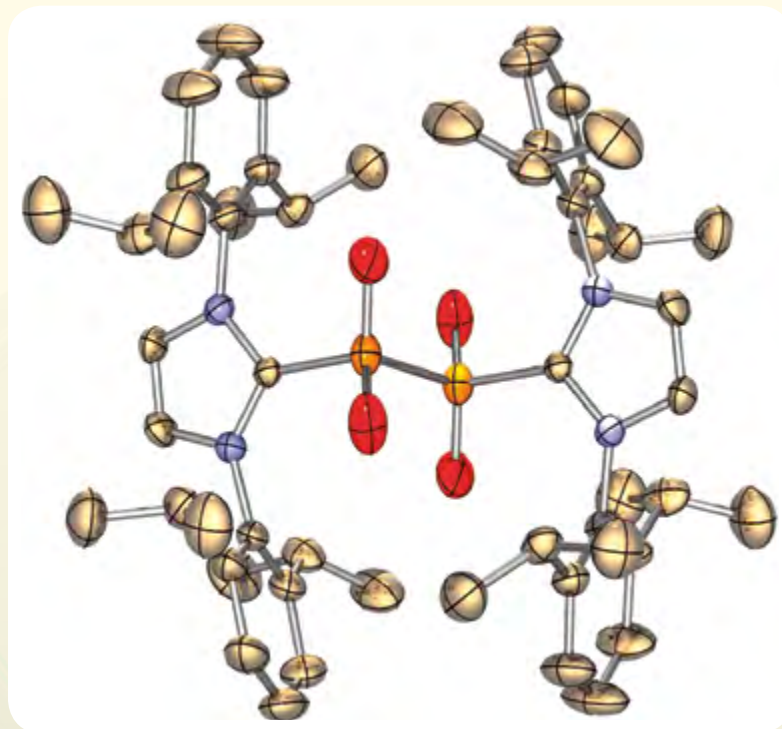
Encouraged by the great physical properties, the group further evaluated the particles in small animal tumor models for tumor targeting and imaging.

For that purpose, the particles were coupled to a tumor recognizing molecule. This grants the particles with the ability to selectively home to tumors from the circulation. Later, *in vivo* MRI studies confirmed the hypothesis: after systemic injection of the carbide nanoparticles, the researchers observed significant signal changes in tumors in MRI images. They also confirmed, by immunostaining, that the signal change was indeed caused by nanoparticle accumulation in tumors. These observations strongly suggest the potential of Fe_5C_2 nanoparticles in MRI as well as other related fields. ●



Jin Xie

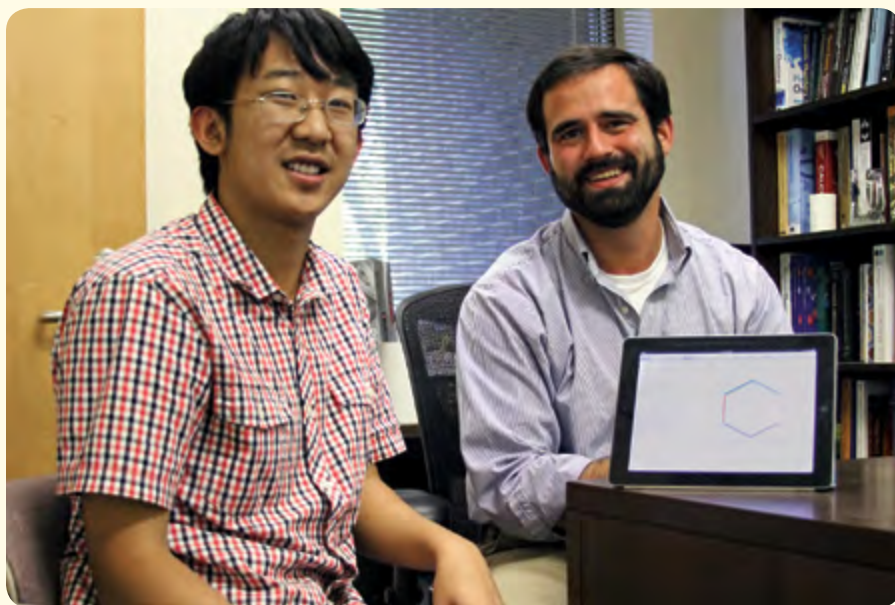
UGA Chemists Split Molecular Oxygen En Route to Diphosphorus Tetroxide



ground state conformation was the asymmetric $\text{O}_2\text{P-O-PO}$ isomer. However, these chemists were able to “trap” this highly reactive molecule in the less stable symmetrical $\text{O}_2\text{P-PO}_2$ isomer. Significantly, this carbene-stabilized diphosphorus tetroxide represents the first example of a phosphorus oxide exhibiting Lewis acid behavior. Robinson believes that this result suggests a new synthetic strategy to probe the chemistry of the highly reactive simple phosphorus oxides. ●

A group of UGA chemists led by Yuzhong Wang and Prof. Greg Robinson have prepared the first stable molecule containing diphosphorus tetroxide, P_2O_4 , via a novel approach involving the reaction of molecular oxygen with the base-stabilized diphosphorus. The base involved belongs to an important class of donor bases known as N-heterocyclic carbenes. Diphosphorus tetroxide is the long-sought phosphorus analog of the rocket propellant N_2O_4 . Although phosphorus lies immediately beneath nitrogen on the Periodic Table, the chemistry of these first two pnictogens could not be more different. For example, while nitrogen gas (N_2) is ubiquitous (making up nearly 80% of the earth's atmosphere), P_2 is transient and generally only observed at high temperatures. Moreover, the chemistry of nitrogen oxides is extensive and well developed while the chemistry of simple phosphorus oxides is considerably less well understood due to their high reactivity. Consequently, simple phosphorus oxides have generally only been studied computationally or in argon matrices. Indeed, UGA computational chemists Yaoming Xie, Paul Schleyer and Fritz Schaefer collaborated with Wang and Robinson on this study. Unlike dinitrogen tetroxide, which has a symmetrical $\text{O}_2\text{N-NO}_2$ ground state structure, computations suggested that the diphosphorus tetroxide

UGA Professor, High School Student Team Up to Create Organic Chemistry App



UGA Young Dawgs summer research program participant Chuanbo Pan (left) and Associate Professor of Chemistry Jason Locklin

The second organic chemistry course a college student takes is often referred to as the “gateway to medical school” because students must learn, synthesize and use knowledge in a rapid fashion to make decisions, much like a doctor.

Jason Locklin, an Associate Professor of Chemistry, knows the subject matter of his class is difficult to master. Despite ample resources—books, notes, lectures and further readings—provided for students, he hears consistent and continued requests from students for more accompanying learning materials.

Now, thanks to the help of recent UGA Young Dawgs summer research program participant **Chuanbo Pan**, who is a neighbor of Locklin and an 11th-grader at North Oconee High School, organic chemistry students at the university and nationwide will have yet another resource at their fingertips—an iPhone and iPad app.

Known as the “Organic Chemistry II Survival Guide,” the application provides easy-to-navigate notes for organic chemistry students and is based on three binders full of Locklin’s teaching materials and notes.

“When I was looking at the available

apps, I realized that there are a lot of apps out there for Organic Chemistry. The problem with these is that I don’t know where the materials come from or the technical background of the people that are making them. Are they experts in Organic Chemistry?” Locklin said.

“I wanted to create an app using my notes that I could verify and have confidence in, so that the students could have the material with them at all times, like when they’re on the bus or waiting to take the test. I wanted to have some new technology at their fingertips to make it easier to access and, hopefully, increase how easy it is to study.”

Locklin read about Pan’s “LatinHelper” app in the Oconee County newspapers and also knew Pan’s father, Zhengwei Pan, an Associate Professor of Physics and Engineering at UGA. Given the high school student’s interest in computer programming, Locklin approached him with the idea of collaborating to create an “Organic Chemistry II” app for students at UGA.

The two worked together, meeting on the weekends over the summer. Pan took hundreds of pages of notes and meticulously diagrammed more than 200 chemical reactions into a format that

could be used in the application.

“In the end, we’ve got a product that we’re both really proud of,” Locklin said. “It contains a tremendous amount of information, and it’s very user-friendly, and, most importantly, I know that the information is accurate.”

Pan included a feature that allows students to draw out chemical reactions themselves, like they would on a sheet of paper, giving them another way to better learn the information. Students can also flag reactions for further review and add text notes.

“You can take notes either using the text editor or you can write with your fingertip, which allows you to draw a reaction out and take notes on it,” Pan said.

“This is really important for organic chemistry because you have to draw molecular structures,” Locklin said. “I think that functionality is really what makes this app unique.”

The resulting application will afford students the opportunity to learn organic chemistry without carrying around large binders of notes and large textbooks.

“Instead of a notebook, or several, you’ve now got almost everything you need to learn with you on your phone or your iPad at all times,” he said. “It is not a substitute for your textbook or lectures, but it has all the reactions and arrow-pushing mechanisms.”

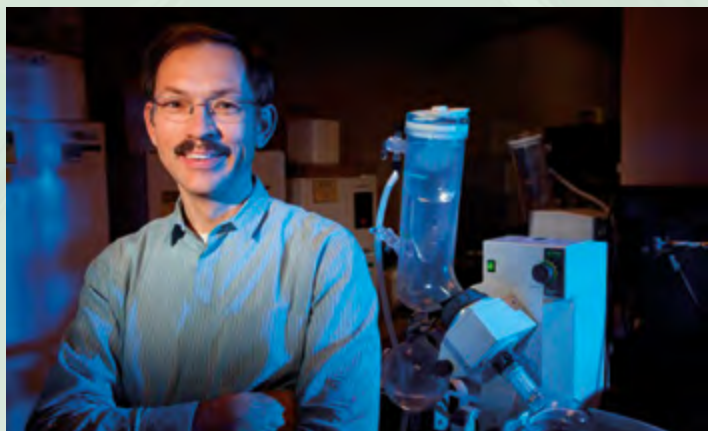
Many of his students are already using iPads and iPhones to take notes in class, Locklin added. “Our goal is to reach you any way possible. Anything that helps you do better in the course or learn the material, I think that it is my job as a professor to be an effective communicator of the material. And I think that’s something that this app allows us to do.”

The “Organic Chemistry II Survival Guide” is \$3.99 for the iPhone app and \$4.99 for the iPad app. To learn more or download the iPhone version, see tinyurl.com/pnn6usv.

To download the iPad version, see tinyurl.com/p4dcbpc.

A video of Locklin and the app in action is available at tinyurl.com/qjkffqd. ●

\$7.4M NIH Grant Will Be Used to Study Building Blocks of Life



Prof. Geert-Jan Boons

A team of senior researchers headed by **Prof. Geert-Jan Boons** has received a five-year \$7.4 million grant from the National Institutes of Health to help better understand one of the most fundamental building blocks of life. They are tiny chains of sugar molecules called glycans, and they cover the surface of every living cell in the human body-providing the necessary machinery for those cells to communicate, replicate and survive. But they're not all good. Glycans support the function of all cells, including those that cause cancer, viral and bacterial infections, diabetes and cardiovascular disorders. This makes them an attractive target for new treatments, and the experiments supported by this grant promise to speed the development of new, more

effective therapies for many of humanity's most insidious diseases and increase understanding of the body's most basic cellular functions.

"We know that glycans are involved in almost every aspect of health and disease, but we need to figure out what controls glycan behavior - the machinery that creates glycans and places them on the surface of cells," said Boons, a Chemistry faculty member and researcher at UGA's Complex Carbohydrate Research Center.

Scientists estimate that there are more than 7,000 unique glycan structures in human cells, but they do not have a strong understanding of the processes involved in creating this vast diversity. Therefore, the UGA team has made identifying and describing the various enzymes that drive glycan formation a central priority of its research.

Co-principal investigator Kelley Moremen has developed a new method to generate these critical enzymes in the laboratory, which the entire research group will use in its experiments. This catalog of enzymes will give researchers new insights into glycan formation and the processes involved in disease development.

"If we can figure out this machinery, we can discover ways to interfere with it, which opens the door for new therapeutics," Moremen said.

The research team is composed of five professors from the Franklin College of Arts and Sciences: Boons, Franklin Professor of Chemistry; Moremen, Professor of Biochemistry and Molecular Biology; James Prestegard, Professor and GRA Eminent Scholar of Chemistry and Biochemistry and Molecular Biology; Richard Steet, Associate Professor of Biochemistry and Molecular Biology; and Lance Wells, Associate Professor and GRA Distinguished Investigator of Biochemistry and Molecular Biology. ●

I N M E M O R I A M



Paul von Ragué Schleyer, 84, a towering figure in Physical Organic Chemistry and a Professor at the University of Georgia since 1998, died at his home in Ila, GA on November 21, 2014. Paul was still actively working, teaching

classes, running his research program, and writing papers up until the day of his death.

Born in Cleveland, Schleyer earned an A.B. in Chemistry from Princeton University in 1951. He then attended Harvard University, where he received an M.A. in Chemistry in 1956 and a Ph.D. in Organic Chemistry in 1957, working under the direction of Prof. Paul D. Bartlett. He returned to Princeton as an instructor and was named Eugene Higgins Professor of Chemistry there in 1969.

In 1976, Paul left Princeton and joined the University of Erlangen-Nuremberg, in Germany, as co-director of the Organic Institute. In 1993 he became founding director of its Computer Chemistry Center. Because of mandatory retirement laws in Germany, he retired from the university as Professor Emeritus in 1998. Schleyer then continued his career as Graham Perdue Professor at the University of Georgia, where he

was a member of the Center for Computational Quantum Chemistry (CCQC).

Delving into a broad range of physical organic, organometallic, inorganic, and theoretical chemistry topics, Schleyer made vast contributions, including discovering ways of synthesizing adamantane and other cage molecules by rearrangement. He also identified new types of hydrogen bonding, elucidated solvolysis mechanisms, and expounded on the nature of reactive intermediates, particularly those of carbocations such as the infamous 2-norbornyl cation. Schleyer discovered many new molecular structures, particularly those involving lithium and electron-deficient systems. Most recently, he focused on nuclear magnetic resonance, aromaticity, and planar hypercoordination of carbon and other elements.

A prolific and highly cited chemist, Paul published more than 1,200 papers. He also authored or coauthored 12 books, some of which involved collaborations with Nobel Laureates Herbert C. Brown, George A. Olah, and John A. Pople.

"Paul Schleyer was a titan among modern chemists," says Peter J. Stang, Professor of Chemistry at the University of Utah and editor of the *Journal of the American Chemical Society*.

"He was one of the few who understood and appreciated and made major, significant contributions to both experimental and computational, theoretical chemistry." ●

During his career, Schleyer "turned to the new computational chemistry and, in cooperation with Pople and others, made it a most significant and active area of chemistry," says Olah, who is a Professor of Chemistry at the University of Southern California. "He never received the recognition he fully deserved for his pioneering work, but future generations will remember him as one of the truly great chemists of our time."

Schleyer received numerous honors. From ACS, he received the James Flack Norris Award in Physical Organic Chemistry in 1987 and an Arthur C. Cope Scholar Award in 1991. He was past president of the World Association of Theoretical & Computational Chemists, coeditor emeritus of the *Journal of Computational Chemistry*, and editor-in-chief of the "Encyclopedia of Computational Chemistry." Schleyer was a fellow of the American Academy of Arts & Sciences and the Bavarian Academy of Sciences. He was a 63-year member of ACS.

CCQC will continue with plans to present a symposium of Schleyer's work on February 11-12, 2015; it had been scheduled to coincide with his 85th birthday. A memorial service was held in the Chemistry Department on Tuesday December 2, 2014.

Schleyer is survived by his wife, Inge, whom he married in 1969; his daughters by his former marriage, Karen Harvey, Betti, and Laura; and four grandchildren. ●

Retirements



Bert and Jim Prestegard at his retirement reception at the CCRC.

James Prestegard

Jim Prestegard retired from UGA on July 31, 2014. He was born in Minneapolis on January 27, 1944, and received his B.S. degree in Chemistry from the University of Minnesota in 1966. He then moved to California to attend graduate school at Cal Tech. While he intended to pursue research in physical organic chemistry, he quickly became fascinated with the biophysical chemistry going on in Prof. Sunney Chan's group and produced a thesis exploring applications of Nuclear Magnetic Resonance (NMR) to both nucleic acids and ion-transport antibiotics under Chan's direction. He joined the Chemistry Department at Yale University as an Assistant Professor in 1970, and was promoted through the ranks there to Full Professor. In 1998, he moved to the University of Georgia as a Georgia Research Alliance Eminent Scholar in the Complex Carbohydrate Research Center, with joint appointments in Chemistry and Biochemistry.

The Prestegard laboratory specializes in the development and application of NMR methods for the study of systems of biological interest. The focus has evolved from lipid membranes to proteins to carbohydrates, and now to combinations of these systems. Prestegard's lab produced its first NMR structure of a protein in 1988 (acyl carrier protein), a structure which stood as the only structure of a fatty acyl carrier protein until a crystal structure appeared in 2001. The lab has produced many protein structures since that time, including one of the first integral membrane protein systems, the glycoporphin dimer, in 1997. In the course of this activity new methodology was developed, including the use of lipid bicelles as an orientable medium for characterizing glycolipids and residual dipolar couplings (RDCs) as a new source of information on protein structure. In 2002 Professor Prestegard, along with Aksel Bothner-By and Ad Bax, was recognized for the introduction of RDCs by the Laukien Prize for outstanding contributions to experimental NMR. Since coming to UGA, Prestegard's interests have turned to glycan-protein interactions and glycoprotein structures. Jim plans to continue to be active in research. ●

Nigel Adams

Nigel G. Adams retired on July 31, 2014 after almost 25 years in the Department of Chemistry at the University of Georgia. He was born in Birmingham, England and received his B.Sc.

in Physics from the University of Birmingham, England in 1963, and an M.Sc. in the Physics of Solids in 1964. He was awarded a Ph.D. in Electron Physics in 1966, also from the University of Birmingham, for his studies of the surface interactions of electrons with insulator single crystals. He was an ESRO/NASA International University Research Fellow at the University of Colorado in Boulder for the period 1968-1969, after which he returned to the UK and the University of Birmingham, moving through the ranks to Senior Research Fellow and Senior Lecturer (the UK equivalent of Full Professor) in the Department of Space Research. In 1978 he was awarded a D.Sc. for his research in Space Physics. In 1990 he moved to the University of Georgia as Professor of Chemistry. In 1995 he became a University Research Professor, and in 2000 he became a Distinguished Research Professor. He was a visiting Erskine Fellow at the University of Canterbury, New Zealand in 1995, and for the period 1999-2000 he was a Program Director for Physical Chemistry at the National Science Foundation. He has been elected to fellowships in the UK Institute of Physics (1984) and the American Physical Society (2004).

In the Adams laboratory, research has concentrated on the fundamentals of gas-phase ionic reaction processes and their application to natural plasmas. This has direct relevance to the interstellar medium (ISM) and to planetary atmospheres. Of particular interest is Titan, a planetary satellite of Saturn, which was visited by the NASA spacecraft Cassini. Its atmosphere is thought to be similar to that of primordial Earth, and thus the chemistry which occurs there is of great interest. To determine the chemical composition of this atmosphere (and indeed of the interstellar medium and of other planetary atmospheres) it is necessary to have laboratory data for accurate and meaningful chemical modeling. For the past forty years, Professor Adams's research has been providing this data, and has led to several key discoveries about the chemistry of the interstellar medium and of planetary atmospheres. To measure pertinent reactions in the laboratory, he was one of two inventors of the powerful Selected Ion Flow Tube (SIFT) method for studying ion molecule reactions under conditions that simulate the low temperature, low pressure plasmas of the ISM. The SIFT is now the technique of choice for examining ion-molecule reactions and has been copied in more than twenty laboratories throughout the world. In the Adams laboratory at UGA, two unique instruments, the SIFT and the flowing afterglow, have been constructed to study individual gas-phase reactions as a function of temperature over the range 70K to 600K (applicable to reactions of planetary atmospheres and the ISM). Professor Adams has also developed and refined the Flowing Afterglow Langmuir Probe (FALP) apparatus, which is used to examine the important process of electron-ion recombination, a key process in the formation of many species of interest in Space Physics. His work has been groundbreaking in the identification and quantification of the neutral products of recombination.

Nigel plans to continue his research as an emeritus professor, focusing on larger species of interests to Titan's atmosphere and to planetary atmospheres in general. ●



Nigel Adams

- 1974 Spencer, Ken**, Chatham, NJ. Ph.D. (w/R. K. Hill). 1975-76 postdoc at U. of Penn (w/M. Cava). Ken worked in chemistry discovery research during 1976-81 at Sandoz (crop protection), 1982 Merck (biocides) and 1983-89 Anaquest (inhalational and IV anesthetics). He worked in clinical research from 1989-2003 at Organon resulting in two FDA drug approvals: Zemuron (rocuronium bromide, Org 9426) and Saphris (asenapine, Org 5222). He worked in clinical quality assurance in 2003-07 at Organon, 2008-09 Schering-Plough, 2010-11 Merck, and is currently in this role at Sanofi Pharmaceuticals. Ken and his wife Marjorie live in northern NJ and enjoy hiking and kayaking at their vacation home in the Pocono Mountains near East Stroudsburg, PA.
- 1990 Ehlers, Charles**, Spartanburg, SC. Ph.D. (w/J. Stickney) Charlie just completed 16 years at Milliken & Company in Spartanburg, SC. After 12 years of managing the corporate analytical lab, Charlie has moved to a technical role in the plastics additives business, supporting new product development, registration, and commercialization. Charlie and family (wife and seven kids) live in Greenville, SC.
- 1999 Reddic, John**, Greenville, SC. Ph.D. (w/ M. Duncan) John recently moved from Columbia, SC to Greenville, where he is now Chemistry Laboratory Technical Director for the Greenville Hospital System. According to John, his work in grad school with lab instrumentation put him in a good position for what he does now, which includes many troubleshooting and instrumentation issues. His wife Mollie is a Methodist minister. Her appointment at her church in Columbia went through May of 2014. She started an appointment in Greenville in June, but John did lots of commuting in the meantime. They are both looking forward to being settled together in Greenville in the fall.
- 2003 Grieves, Greg**, Atlanta, GA. Ph.D. (w/M. Duncan) Greg had a kidney transplant in 2013 and is doing very well after a previous period of serious illness. He got married in October of 2013, and his wife Carla is a social worker in Atlanta. After working as a Research Scientist at Georgia Tech for over 10 years, Greg recently took a job as a "configuration engineer" with HealthPort, developing software for medical records. He visited Athens for a Physical Chemistry Seminar on his research on August 29. Greg and Carla just bought a house in Sandy Springs, GA.
- 2003 Mathe, Mkhulu, (aka Kenny)**, Gauteng, South Africa. Ph.D. & Postdoc (w/J. Stickney) Mkhulu is a proud grandfather of a year old boy, whose mother and husband will celebrate their first anniversary in October. His youngest daughter, age 6, has started playing golf at school. Mkhulu currently works for the Council for Scientific and Industrial Research in the Energy Materials competence area.
- 2004 Whiteside, Tad**, Aiken, SC. Ph.D. (w/L. Carreira) Tad Whiteside was chosen to receive the Erskine College Outstanding Young Alumnus Award for 2014. Winners are selected by the alumni board; the Award recognizes alumni from the last 15 years who have had a positive influence in service to their community, church, profession and Erskine. Tad attended Erskine from 1996-2000, where he graduated with a B.S. in Chemistry and a B.A. in Physics, with a minor in Mathematics. At Georgia, he worked with Prof. Butch Carreira, studying physicochemical properties of organic compounds, and received his Ph.D. in Physical chemistry in 2004. After a postdoc at the U.S. E.P.A. in Athens, Tad accepted a position at the Savannah River National Lab in Aiken, SC, where he works in the Environmental Restoration Technologies section and assists in performance assessment modelling. He recently completed a term as Chair of the Savannah River Section of the ACS.
- 2005 Kishore, Anita**, New York, NY. Ph.D. (w/J. Prestegard) After graduating from UGA Chemistry in 2005, Anita began consulting at Bain & Company in San Francisco and Munich, advising clients in pharmaceutical and biotech companies in strategy and operations, including portfolio selection, new product development, and R&D design and operations, as well as helping Bay Area science and technology museums raise funds. She joined Sandoz in 2010, the division of Novartis that manufactures generic pharmaceuticals, and developed global strategy from headquarters in Holzkirchen, Germany. Anita returned to the New York City area a couple of years later to lead US Portfolio Management for Sandoz and eventually to join Pfizer as a Senior Director of Strategy & Innovation, working on commercial strategy for primary care products. Anita recently left Pfizer to focus on a lifelong passion of increasing access to medicines for patients in developing countries by interning at Doctors Without Borders/ Medecins Sans Frontieres and now as a Manager of Vaccines Cold Chain Logistics at the Clinton Health Access Initiative. Anita served on the board of the Global Freedom Center, a non-profit dedicated to fighting human trafficking, and loves to cook, run, and listen to live music in her spare time.
- 2005 Page, Michelle**, Marietta, GA. B.S. (w/C. Kotal). Michelle went to Indiana University in Bloomington for graduate school. She left with her masters and started instructing at Kennesaw State University. She moved on from instructing to be an analytical chemist at a small testing laboratory in Marietta, GA and has now found her way to Leco Corporation as a new Sales Engineer for their Separations Sciences Division for the southeast territory working primarily with GC-TOF-MS. Michelle is married with a beautiful two year old son!
- 2008 Molek, Karen (Sinclair)**, Pensacola, FL. Ph.D. (W/ M. Duncan). Karen is Assistant Professor at the University of West Florida. She and co-PI Prof. Michael Huggins, were recently awarded an NIH National Institute of General Medical Sciences Maximizing Access to Research Careers for Undergraduate Student Training in Academic Research (NIH NIGMS MARC U-STAR) in the amount of \$930,000. This grant will establish a MARC Scholars program at UWF for 2014-2019 to provide support for underrepresented undergraduate students pursuing Ph.D. or M.D./Ph.D. degrees in the biomedical and behavioral sciences.
- 2008 Kim, Jay**, South Korea. Ph.D. (w/J. Stickney) Jay is currently a research professor in the Department of Chemical Engineering and Materials Science at Hanyang University, Ansan, South Korea. His son, Alex, will be in elementary school next year.
- 2008 Velasquez, Joe**, Los Alamos, NM. Ph.D. (w/M. Duncan) Joe is a postdoc at Los Alamos National lab, working on a laser cooling project. To laser cool CaH (which he is working on currently), it takes four co-propagating mode-locked lasers that each have frequency shifts in the neighborhood of 200-500 MHz (using AOMs). No other lab is presently attempting to do direct laser cooling of a molecule like this, so he has had to fully characterize the laser vaporization source used to produce the CaH. Xe is used as a carrier to give the slowest terminal velocity in the molecular beam before laser cooling begins.
- Lisa and Joe love it in the northern NM area. Joe spends much of his time in the lab, but Lisa has become a fly fishing guide (part time). They try to make it up to the mountains once a month together, but most weekends she is with clients or scouting. Lisa's day job is as the office manager for a medium-sized construction company here in northern NM. Joe's present contract with the lab officially terminates September 30, but he is hoping to get a permanent staff position, depending on the funding situation.
- 2010 Ricks, Allen**, Chico, CA. Ph.D. (w/M. Duncan) Allen has recently left his position with Ultrafast Systems in Florida, and started as an Instructor of Chemistry at California State University-Chico this fall, where he is teaching undergraduate Physical Chemistry.
- 2011 Pierce, Wendy**, Memphis, TN. Ph.D. (w/J. Prestegard) Wendy left the Prestegard lab at UGA in May 2011 to start a Postdoctoral Associate position with Dr. Tanja Mittag at St. Jude Children's Research Hospital in Memphis, TN. In the Mittag lab, her project involved elucidating the mechanism of two multivalent proteins, Gli3 and SPOP, and how they interact using biophysical techniques that include Nuclear Magnetic Resonance, Analytical Ultracentrifugation, and Fluorescence Polarization. Gli3, a transcriptional factor in the Hedgehog (Hh) signaling pathway, is regulated through ubiquitination and degradation via SPOP mediated recognition. Deregulation of either of the proteins can lead to cancers or Gli3 developmental disorders. Understanding the mechanism of interaction would provide targeted therapies for associated diseases. After a little over three years of being in the Mittag lab, she is leaving to take a Project Coordinator position still at St. Jude. In this position, she will be establishing and tracking project timelines and milestones for a multi-institutional team working to find new drug therapies for pediatric ependymoma from preclinical to clinical studies. She will be collecting and integrating data from project team members and other sources to maintain an organized project environment. Overall, the research teams involved aim to find the best personalized treatments and cures for the

- disease for the patients. During her tenure at St. Jude, she has really enjoyed being part of this organization that goes far and beyond, to reach Danny Thomas' (the founder) dream that "No child should die in the dawn of life."
- 2012 Bandyopadhyay, Biswajit**, Berkeley, CA. Ph.D. (w/M. Duncan) Biswajit is working at the Chemical Dynamics Beam Line at the Advanced Light Source, Lawrence Berkeley National Lab, with Dr. Musa Ahmed. On June 20, 2014, he was married to Anandi Roy (present UGA graduate student) in San Francisco, with many family members attending.
- 2012 Lu, Aaron**, Ewing, NJ. Ph.D. (w/H. Schaefer) Aaron has accepted a permanent position at the Universal Display Corporation in Ewing, NJ and began in September of this year.
- 2012 Sontag, Kyle**, Minnesota. Ph.D. (w/J. Locklin) Kyle is working hard every day as a Senior Materials Scientist at Donaldson.
- 2013 Brathwaite, Antonio**, St. Thomas, Virgin Islands. Ph.D. (w/M. Duncan) Antonio started a position as Assistant Professor (tenure track) at the University of the Virgin Islands in August. His wife Tamika is serving as a clerk for a federal judge in St. Thomas. Antonio hopes to be able to come back to Athens in the summers to bring undergraduates to the Duncan group for research.
- 2013 Compaan, Katie**, Potchefstroom, South Africa. Ph.D. (w/H. Schaefer) Katie got married to Garth Randall in summer 2013. They just had a beautiful baby daughter Sarah, and Katie is now a faculty member at the North-West University, Potchefstroom, South Africa.
- 2013 Hargis, Jacqueline**, Tampa, FL. Ph.D. (w/H. Schaefer) Jacqueline begins her job next month with Xcellence; a Pharma company near Tampa, Florida, Jacqueline's much loved home town.
- 2013 Hollman, David**, Livermore, CA. Ph.D. (w/H. Schaefer) David has accepted a permanent position at the Sandia National Laboratories in Livermore, California and began work there in mid-September of this year.
- 2013 Mosley, Jonathan**, Athens, GA. Ph.D. (w/M. Duncan) Jonny graduated in the summer of 2014. He has just received a National Research Council Postdoctoral Fellowship and began work in September at the U. S. EPA Laboratory in Athens, working with fellow UGA alumnus Tim Collette (Ph.D. w/ Carreira).
- 2013 Narendrapurap, Beulah**, Statesboro, GA. Ph.D. (w/H. Schaefer) Beulah is now a Lecturer at Georgia Southern University.
- 2013 Tierney, Megan**, Hattiesburg, MS. B.S. Megan began medical school in the fall of 2014 at the William Cary University School of Osteopathic Medicine.
- 2013 Vogt, Stefan**, Santiago, Chile. Ph.D. (w/H. Schaefer) Stefan is now a postdoc with Professor Alejandro Toro-labbe at the Catholic University in Santiago, Chile.
- 2013 Young, Justin**, Albuquerque, NM. Postdoc (w/M. Duncan) Justin has just begun a postdoctoral position at the Air Force research Lab in Albuquerque, working with Dr. Jaime Stearns.
- 2014 Althoff, Ashley**, B.S. Ashley will be traveling Europe for part of the summer and plans to attend Medical School in the fall.
- 2014 Arnold, Rachelle**, Bainbridge, GA. Ph.D. (w/J. Locklin) Rachelle has accepted a Research Scientist position at DaniMer Scientific, LLC, in Bainbridge, GA.
- 2014 Badel, Erik**, B.S. Erik will perhaps pursue pharmacy school or some other post-graduate schooling.
- 2014 Bagget, Mary Caitlin**, B.S. Mary will be applying to Pharmacy school next year for the class of Fall 2015, and during her year off, she will gain work experience in industry.
- 2014 Beck, Meredith**, Atlanta, GA. B.S. Meredith applied to medical schools this summer. She worked last summer as a guest researcher at the CDC Birth Defects Branch.
- 2014 Christie, Malika**, B.S. Malika plans to apply to Dental School for the fall 2015 semester.
- 2014 Croft, Brian**, B.S. Brian will be working as a research assistant at Georgia Regents University while he applies to Medical School.
- 2014 Dibble, Michael**, B.S. Michael will continue his research while applying to Ph.D. programs in chemistry. During his Ph.D. studies, his ultimate research goal will be to study the organic and bio-inorganic basis of Parkinson's disease.
- 2014 French, Robert**, B.S. Robert plans to pursue a career in Dentistry and work in industry during the application process.
- 2014 Fultz, Zachary**, B.S. When asked about his future plans, Zachary said "I plan to enter the workforce in industry to support my wonderful fiancée."
- 2014 Grayeski, Philip**, B.S. Ultimately, Philip wants to develop advanced therapeutics, particularly nucleic-acid based therapeutics, and translate these technologies into a small biotech company and viable options for patients who suffer from a variety of hereditary diseases.
- 2014 Hamilton, Anthony**, B.S. Anthony plans to travel and visit prospective universities to find a suitable Ph.D. program in Chemistry.
- 2014 Heying, Elizabeth**, B.S. Elizabeth attended classes in the summer to earn her Masters of Arts in Science Education. Her future plan is to be a high school science teacher.
- 2014 Hodges, Holly**, B.S. Holly plans to pursue a career in the cosmetics industry as a research chemist.
- 2014 Huseman, Tyler**, B.S. Tyler will attend the University of Georgia School of Law and pursue a degree in Patent Law. He hopes to specialize in pharmaceutical patent law. Tyler traveled to Panama and Spain this summer.
- 2014 Maddox, Brett**, B.S. Brett was accepted to Georgia Regents University College of Dental Medicine for the fall 2014 semester.
- 2014 Martin, Meredith**, B.S. Meredith's immediate goals are to apply to and attend medical school.
- 2014 McGill, Martha**, B.S. Katy plans to work for a year in industry before attending the University of Florida to earn a Ph.D. degree in Chemistry.
- 2014 Norris, Isaiah**, B.S. Isaiah plans to work in industry and is getting married in May of 2015.
- 2014 Rivera, Shannon**, B.S. Shannon has been accepted into Emory University's Ph.D. program in Biomolecular Chemistry.
- 2014 Ruddick, Caitlin**, B.S. Caitlin Plans to attend medical school to become either a transplant surgeon, an oncologist, or an emergency room physician. She is taking a gap year in order to work as a medical assistant for a skin cancer specialist.
- 2014 Schuldt, Kim**, Gaithersburg, MD. M.S. (w/G. Smith) Kim is now working at the National Institute of Standards and Technology (NIST).
- 2014 Schwartz, Nichole**, B.S. Nichole will pursue the Ph.D. degree in Chemistry at the University of Virginia.
- 2014 Sims, Mark**, B.S. Mark began a career in the chemical industry this summer.
- 2014 Thompson, Tristin**, B.S. Tristin also studied Food Science as an undergraduate and enrolled this Fall in the Master's program in Food Science here at UGA.
- 2014 Walker, Orrett**, B.S. Orrett's immediate plans are to seek research opportunities at the Center for Disease Control in Atlanta, GA.
- 2014 Watson, Jr., Timothy**, B.S. Alan plans to attend graduate school for chemical engineering starting fall 2015.
- 2014 Webster, Ian**, B.S. Ian's immediate plans are to travel the world for one year prior to applying to graduate school in Chemistry.
- 2014 Welsh, Travis**, B.S. Travis began Medical School this fall. He traveled this summer across the United States.
- 2014 Xie, Wenbo**, B.S. Wenbo took a backpacking trip around South-East Asia this summer.
- 2014 Yau, Kimberly Han-Ming**, B.S. Kimberly will attend medical school at the University of Virginia. ●



Rich Steet, Mike Terns, Carl Terns, Bob Sabatini

2014 Chemistry Golf Scramble

The 2014 Chemistry Golf Scramble took place at the UGA Golf Course on Saturday April 19. In spite of a rainy day, the golfers played on and had a great time. The afternoon golf was followed by a barbecue, sponsored by the Chemistry Department. The team of Rich Steet, Mike Terns, Carl Terns, and Bob Sabatini shot an impressive score of 64 to win, followed closely by the second place team of Dudley Christie, David Ladner, Mike Duncan and Richard

Calendar of Events 2014-2015

(see departmental web site for more details)

- February 12, 2015 **Paul Schleyer Memorial Symposium**
- April 17, 2015 **Alumni Appreciation Lecture and Banquet/Awards Night**
- April 18, 2015 **Golf Tournament**
Saturday, UGA Golf Course
- Fall 2015 **Allinger Lecture**

Walters, who shot a 65. Bob Scott won the putting competition that took place on the putting green after the round. Alumnus David Ladner won the longest drive competition on hole number 18, and Mark Ebell won the closest-to-the-pin shot on hole number 13. Alumni players included Dudley Christie, David Ladner, Jeff Sherman, Jonathan Anderson, Sean Marrache, Mickey Kinley, Tad Whiteside and Richard Walters. ●

Send us your updates on new jobs, marriages, children, retirements, special trips, etc. to Lauren Bowman at head@chem.uga.edu, or call 706-542-1919. We are especially interested in receiving your email addresses, so that we can send out reminders about upcoming events.

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