

2013-2014  
Annual Report

Submitted to the College of Arts & Sciences

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Chair, Department of Chemistry

# **ANNUAL REPORT**

Department of Chemistry  
College of Arts and Sciences  
The University of Alabama

For the Period  
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## One Page Summary

**Faculty Appointments:** Dr. Elizabeth Papish joined the faculty as an associate professor in fall 2013. Dr. Papish is an inorganic chemist and comes to UA from Drexel University. Dr. Laura Busenlehner and Dr. Shanlin Pan were awarded tenure and promoted to associate professor effective in fall 2014. Dr. Kevin Shaughnessy was promoted to full professor. Dr. Shaughnessy also was reappointed as chair through the 2018-19 academic year.

**Awards:** Faculty: Dr. David Dixon was named a Fellow of the American Chemical Society in recognition of his many contributions to the field of chemistry and his long service to the ACS. Dr. Arun Gupta received the Chemistry Research Society of India (CRSI) Medal, which is presented to Indian chemists working outside of India for their contributions to the field of chemistry. Dr. Robin Rogers received the Paul Linden Award in Ionic Liquids from German Science Foundation Priority Program on Ionic Liquids. Graduate Students: Dr. Mier An received the College Outstanding Dissertation award and Mingyang Chen received the College Outstanding Dissertation Research Award. Michele Stover and Steven Kelley were chosen to attend the Lindau Nobel Laureates meeting in summer 2013.

**Teaching:** The Chemistry Department accounted for over 26,000 student credit hours, which was a 13% increase over AY 12-13. The median faculty member was responsible for 781 SCH during the academic year. The department had 206 undergraduate majors and 97 PhD students in 13-14. The department had 20 BS, 10 MS, and 10 PhD graduates in 2013.

**Research:** Department faculty have over \$13 million in current funding and received \$3.2 million in new funding during this academic year. The new funding is a 45% increase over 2012-13. Research expenditures totaled \$3.3 million in FY 14. The faculty submitted 104 proposals with a combined requested amount of \$28 million. The faculty published 128 peer-reviewed papers. In addition, the faculty published 22 patent applications, 7 issued patents, 1 book, and 13 book chapters. Chemistry faculty and students presented 180 talks at local, regional, national, and international scientific meetings and 52 invited seminars at other universities or companies.

**Service:** Department faculty provide service to the institution by serving on numerous Department, A&S and UA committees. Drs. Vincent and Blackstock serve on the Faculty Senate and Dr. Cassady serves as an alternate senator. Dr. Rogers is director of the Center for Green Manufacturing. Dr. Vincent serves as chair of the Biological Safety Committee and vice-chair of Institutional Animal Care and Use Committee. Dr. Nikles is the director of the Central Analytical Facility and serves as chair of the CAF Users Advisory Board. Chemistry faculty serve on numerous external committees and are members of 23 editorial or advisory boards for scholarly journals. Dr. Robin Rogers is the editor-in-chief of the journal *Crystal Growth and Design*. Dr. David Dixon serves as Councilor for the ACS Division of Fluorine Chemistry

**Outreach:** Department faculty are actively engaged in outreach activities. Dr. Martin Bakker hosted the week-long Materials Camp for 22 high school and middle science teachers from Alabama and Mississippi. The Office of Naval Research through ASM International Education Foundation, the Office of Academic Affairs, the College of Arts and Sciences and Tuscaloosa City Schools provided funding for the camp. Dr. Laura Busenlehner organized the Diversity Awareness Symposium, which hosted over 70 students from UA and regional colleges. The symposium was sponsored by Dr. Busenlehner's NSF CAREER award. Twelve undergraduate students from around the country participated in the 2013 Research Experience for Undergraduates program, which is funded by NSF.

## I. Full-Time Faculty Highlights

Listed below are paragraphs provided by each faculty member describing his/her highlights for the year. Some of the key highlights are summarized here. Data on research and teaching productivity are collected in later sections of this document.

**Faculty Hiring and Appointments:** Dr. Elizabeth Papish joined the faculty as an associate professor in fall 2013. Dr. Papish came to UA from Drexel University, where she was an associate professor. Dr. Papish's research interests are in the area of inorganic chemistry. Dr. Laura Busenlehner and Dr. Shanlin Pan were awarded tenure and promoted to associate professor and Dr. Kevin Shaughnessy was promoted to full professor effective for the 2014-15 academic year. Dr. Shaughnessy also was reappointed as department chair through the 2018-19 academic year.

**Faculty Awards:** Dr. Anthony Arduengo was awarded a Weidereinladung (Reinvitation) Senior Research Prize by the Alexander von Humboldt Foundation. Dr. David Dixon was named a Fellow of the American Chemical Society in recognition of his many contributions to the field of chemistry and his long service to the ACS. Dr. Arun Gupta received the Chemistry Research Society of India (CRSI) Medal, which is presented to Indian chemists working outside of India for their contributions to the field of chemistry. Dr. Robin Rogers received the Paul Linden Award in Ionic Liquids from German Science Foundation Priority Program on Ionic Liquids.

### Faculty Highlight Paragraphs:

**Dr. Anthony Arduengo** – Professor Arduengo continues to represent UA interests with international funding agencies including Alexander von Humboldt Foundation in Germany with which he holds the post of *Humboldtian on Campus* and functions as an ambassador between The University and The Foundation. Additionally, Professor Arduengo continues as a contact point for UA with the German Academic Exchange Service (DAAD, Deutscher Akademischer Austausch Dienst). Over the past year Professor Arduengo facilitated the student exchange visits of 2 undergraduates in Chemistry at UA in Universities in Germany and Japan, and international visiting scholars in his own laboratory. Together with Professor Till Opatz at the University of Mainz (Germany), Professor Arduengo has laid the ground work for a bidirectional student exchange program between Mainz and Tuscaloosa with the first German students scheduled to arrive in Tuscaloosa in 2015. Professor Arduengo founded a charitable startup company, *Innovative Valency*, that operates to provide funds for research and scholarships through the sale of rare and fine chemicals to R&D laboratories. *Innovative Valency* is off to a strong start with a partnership with a German company, *InnoChemTech*, and now has product listings with the leading chemical databases. Professor Arduengo represents UA prominently on the international stage. Work from his research group continues to appear in highly visible journals world-wide, including a Shelby Hall inside cover article with the prestigious German journal, *Angewandte Chemie*. In January 2014, he was the awardee of an Alexander von Humboldt “Wiedereinladung” grant. He also was selected to deliver the April 2013 Charles M. Knight Lectureship at the University of Akron. Professor Arduengo was the keynote lecturer both the Iminium Salts Conference (ImSAT-11) in Goslar, Germany, and the Heron Island Conference on Reactive Intermediates in Queensland, Australia.

**Dr. Martin Bakker** - saw the granting of a US patent for methods of making hierarchically porous metal and metal oxide monoliths and the filing of a second patent on hierarchically porous carbon supports for precious metal catalysts. This year also saw the graduation of Drs. Amy Grano and Franchessa Sayler. Dr. Sayler is co-founder and majority owner of ThruPore Technologies, which was founded to commercialize patents developed in our group. ThruPores is currently funded by a Phase 1 SBIR grant from the National Science Foundation.

**Dr. Silas Blackstock** - has supervised 4 graduate students (Melody Kelley, Carl Saint-Louis, Chinenyeze (Izzy) Nwankwoala, and David Warner) and 4 undergraduate students (Travis Atchley, Johan Both, Savannah Reach, and Lauren Hagler). Melody Kelley completed her NSF Doctoral Fellowship and was awarded an SREB Dissertation Fellowship to fund her final year in the program. Johan Both graduated in May 2013 and now attends the PhD chemistry program at Stanford University. Dr. Blackstock continued with Dr. Woski the co-direction of the chemistry GAANN program (\$528,608) that funded 7 chemistry PhD students in 2012-13 and a total of 17 annual fellowships for 15 chemistry graduate students (including 9 female, 3 African American, and 1 American Indian students) from 2010-2013. The final report for the chemistry GAANN program has been filed and accepted by the DoEd. In the research laboratory, the group continues to develop redox auxiliary catalysis as a new way to activate and trigger organic reactions. Nine presentations of our research were given in the past year, including a talks and posters at the Spring 2013 and 2014 National ACS meetings in New Orleans and Dallas and 4 research presentations were given locally by Dr. Blackstock and his students.

**Dr. Marco Bonizzoni** - In the last academic year Dr. Bonizzoni submitted multiple major external grant applications, including submissions to the NSF's CAREER program and to the National Institute of Justice Basic Science Program for a total request close to \$1.5m. Dr. Bonizzoni oversaw research on the binding of small molecules onto hyperbranched polyelectrolytes carried out by his two graduate students and postdoc. Dr. Bonizzoni designed and taught a new class in Spring 2014, CH 635 - Supramolecular Chemistry. The class was well-attended and it successful blended traditional frontal lectures with flipped-classroom techniques (for instance, student presentations were used as a final assessment tool for the class; students were involved in the discussion and evaluation of such presentations as well). During the last year, Dr. Bonizzoni served on the Graduate Recruiting Committee for the Chemistry Department, on the Faculty Technology Committee for the College of Arts and Sciences, and on the University Technology and Learning Committee. Dr. Bonizzoni also served as a manuscript peer reviewer for a number of eminent journals including the Journal of the American Chemical Society, the Journal of Organic Chemistry, Chemical Communications; and for funding applications for the NSF.

**Dr. Michael Bowman** - The Bowman group continues its work on the structure and function of enzymes that carry out complex chemical reactions. One project on nitric oxide synthase was completed and a new project on high resolution structure determination in P450 enzymes was started. Individual hydrogens in the P450 or molecules bound to are seen with atomic resolution, determining how drugs that target specific diseases bind to the P450s of humans and disease causing organisms. The result of this research will accelerate the discovery of new drugs to treat a wide range of diseases. Research on the chemistry and properties of trityl free radicals is developing new materials to enhance the sensitivity and resolution of MRI imaging methods.

The Bowman group is helping organize the 43<sup>rd</sup> Southeastern Magnetic Resonance Conference at UA in October. This annual conference will bring students and researchers from colleges, universities and research labs in the southeast together at UA to discuss the latest results and methods for studying problems in chemistry, biomedicine, materials, magnetism and molecular imaging. This conference was last held at UA in 2007 and provides a unique forum to showcase UA and attract undergraduate and graduate students.

**Dr. Laura S. Busenlehner** - Research in the Busenlehner group is focused on the structure and function of metalloproteins involved in human health and includes four Ph.D. graduate students and three undergraduate students. Her group hosted two summer undergraduate research interns during Summer 2012 (*NSF-REU Summer Research Experience for Undergraduates* program and *Howard Hughes* program and has sponsored one *Emerging Scholars* research student throughout the academic year. Research was supported via an NSF CAREER grant, awarded in 2009. Two research papers were published in leading biochemistry journals. The collaborative work published in the *Journal of Biological Chemistry* was chosen as "Paper of the Week" and highlighted in the publication. Dr. Busenlehner also published a book chapter on hydrogen/deuterium exchange mass spectrometry in the well-known *Methods in Molecular Biology* series. Busenlehner collaborates with professors from the Departments of Chemistry and of Biological Sciences at The University of Alabama, and with professors at several notable universities, both domestic and international. Dr. Busenlehner gave invited research presentations at the International Conference on Fe-S Cluster Biogenesis and the Mississippi Regional Biophysical Consortium meeting. Students presented posters in the above conferences, but also the American Chemical Society national meeting and the University's Undergraduate Research conference. Dr. Busenlehner gave invited research presentations at Murray State University, Auburn University, University of Southern Mississippi, and Alabama Local Section of the American Chemical Society. Professor Busenlehner was chosen to serve on the Editorial Advisory Board of the ACS journal *Biochemistry*. She is also on the advisory boards for *Tide Together* and *WiSE* (Women in Science) programs. Prof. Busenlehner serves on the Department of Chemistry Undergraduate Committee (30+ advisees), the Executive Committee and was the chair of the 2013 *Diversity Awareness Symposium* organizational committee, which was held in April 2013. She also is the faculty sponsor for the UA Student Chapter of the American Chemical Society. Dr. Busenlehner has also served as a faculty mentor for the *Tide Together* program and led two workshops on effective presentation skills and scientific writing. She continues to review grant proposals for the National Science Foundation (NSF) and manuscripts for *Biochemistry*, *Journal of Molecular Biology*, and *Journal of Mass Spectrometry*.

**Dr. Carolyn Cassady** – Dr. Cassady's group continued their research efforts involving fundamental and applied mass spectrometry of deprotonated peptide ions and metallopeptide ions. Five graduate students are in the group. In the past year, several presentations of this work were given at the 61<sup>st</sup> Annual American Society for Mass Spectrometry conference in Minneapolis and the Southeast Regional American Chemical Society Meeting in Atlanta. During the past year, the group has been very fortunate to receive new funding from both NSF and NIH. The NSF funding is a renewal of a grant dealing with the gas-phase acidities of acidic amino acids and peptides and the effects of deprotonation site on peptide fragmentation by mass spectrometry. This is a joint experimental and computational project that also involves the

research group of Professor David A. Dixon. The new NIH grant involves the use of metal ions as enhanced protonation and cationization reagents in electron-based dissociation mass spectrometry processes for acidic peptides. The overall goal of both the NSF and the NIH projects is to develop new techniques that can be used by proteomics researchers for the sequencing of acidic peptides, which are difficult to sequence by “conventional” mass spectral techniques. The group also has a new joint project underway with Dr. Yuoping Bao, of the Department of Chemical and Biological Engineering, and Dr. Qiaoli Liang, manager of the UA mass spectrometry facility. This research involves the development of iron oxide nanoparticles as matrices for matrix-assisted laser desorption ionization (MALDI) mass spectrometry. Preliminary results have been obtained with funding from a College Academy of Research, Scholarship, and Creative Activity (CARSCA) grant through UA’s College of Arts and Sciences. A proposal has been submitted to NSF regarding the use of these matrices for organic polymer analysis and the matrices have been the subject of a patent application. Dr. Cassady’s teaching assignment in Fall 2013 was CH 223, Quantitative Analysis. In Spring 2013, she taught the graduate course CH 627, Mass Spectrometry, to a class of 10 graduate students. She was also very involved in service activities. She continued her work as faculty supervisor for the mass spectrometry facility and served on the search committee for UA’s Vice President for Research position. In addition, she is working closely with students to get the new UA-Tuscaloosa Association for Women in Science affiliate group up and running. In November 2013, President Bonner hosted a well-attended reception for the group at the President’s Mansion. Dr. Cassady is also chair of the departmental Retention Tenure and Promotion (RTP) Committee.

**Dr. David Dixon** – During the 2013-2014 academic year, Dr. Dixon was involved in a variety of research, teaching, and service activities. He taught CH-341 Physical Chemistry in the Fall 2013 semester and developed an assessment program as this was the first time he had taught this course. He also taught CH-549, Advanced Physocal Chemistry II, Atoms and Molecules at the same time. A complete set of course notes was developed and handed out to the students due to the limited board space in the lecture room. With continued HHMI funding, he designed a number of new laboratories for CH-117 (Honors Introductory Chemistry) including a Millikan oil drop experiment and a Franck-Hertz experiment. New equipment was purchased for these experiments. These laboratories will be integrated into the course in Fall 2014 semester. He ran the computational chemistry lab for CH-117 in Fall 2013 and will purchase a new computer using HHMI funds to support the laboratory and undergraduate research in summer 2014. He taught a Freshman Learning Community on Energy and the Environment in Fall 2013. He has been active in providing a research experience for undergraduate students through the UA Computer Based Honors Program, undergraduate chemical research, and UA’s emerging Scholars program. He mentored 2 CBHP students and 2 undergrad research students during the Fall 2013 semester and 3 CBHP students, 2 undergrad research students, and 2 Emerging Scholars in the Spring 2014 semester. He mentored 1 undergraduate in his laboratory in Summer 2013 on a DOE funded project. His students received 2 UA Randall Research Awards in April 2014 and one student, Meredith Rickard, received the Randall Scholarship in April 2014. Josh Moon received the Catherine J. Randall Award. Dixon served on the Departmental Undergraduate Committee, advised undergraduate students, served on the 2014 CBHP selection committee, served on the Departmental Long Range Planning Committee, served on the Departmental Safety Committee, served on the UA’s Burnum Award Committee, and provided input to the 2013 Bioinformatics Search Committee for the Biology Department and to the Dean



of the Graduate School on the SEC Faculty Award. He was the Chair of the A&S Technology and Research Working Group. He serves as the sole ACS Councilor for the Division of Fluorine Chemistry and is a member of the Division Executive Committee. He is on the Advisory Board of the *Journal of Physical Chemistry* and the Editorial Boards of *The International Journal of High Performance Computing* and the *Journal of Fluorine Chemistry*. He is on the User Executive Committee of the William R. Wiley Environmental Molecular Sciences Laboratory at PNNL and the User Advisory Board of the Argonne Leadership Computing Facility. He serves as a reviewer for many journals as well as funding agencies. In 2013-2014, the research group had 8 graduate students and up to 4 post-doctoral fellows. Mingyang Chen (August 2013), Virgil Jackson (December, 2013), and Zongtang Fang (May, 2014) received PhD degrees. Jackson is currently a postdoctoral fellow and Chen was one for 2 months. Fang will be a postdoc in the group while his wife finishes graduate work here. There are two DOE Office of Science grants in catalysis (through PNNL and UC-Davis), one in geochemistry/CO<sub>2</sub> sequestration, and one in heavy element chemistry (through ANL). There is a DOE/EERE grant in the area of chemical hydrogen storage led by Boston College. A SBIR Phase II grant with Sentient Corp to support work in hydrogen storage/release for Redstone Arsenal is being completed. The experimental work is being done by the Street group. An NSF grant with C. Cassady as PI for studies of peptide anions for proteomics is in place as is an NSF grant with K. Shaughnessy on homogeneous catalysis. A grant on using frustrated Lewis acid-base pairs has been funded from an LANL LDRD project. Funding from an ANL LDRD project on inorganic synthons was completed. An ANL LDRD grant on the parallelization and parameterization of semiempirical molecular orbital (SEMO) methods was funded and supports a postdoc at ANL as well as staff.

**Dr. Patrick Frantom** - Over the 2013-2014 academic year, Dr. Frantom's laboratory supported five graduate and four undergraduate researchers. During this year, two graduate students were supported on funding from an NSF CAREER Award, and funding from an NSF Graduate Research Fellowship supported a third student. Undergraduate research support came from the Emerging Scholars program and dedicated funding from the NSF CAREER Award. The laboratory published two peer-reviewed publications in the ACS journal Biochemistry, with one article as a Rapid Report, and submitted an additional article currently in revision. Research from the Frantom laboratory generated seven poster and two oral presentations at regional and national conferences with Dr. Frantom receiving an invitation to give an oral poster talk at the 2014 Gordon Research Conference on Isotopes in Chemistry and Biology. Dr. Frantom gave invited lectures at Louisiana State University, Auburn University, Mississippi State University, and Penn State University. Dr. Frantom served as a mentor for the Active Learning Initiative sponsored by the College of Arts and Sciences. Dr. Frantom was also awarded a Distinguished Teaching with Technology Fellowship from the college.

**Dr. Daniel Goebbert** - The Goebbert group currently consists of 4 graduate students and 5 undergraduate students. In the last academic year the group published several manuscripts and presented results at the national American Society for Mass Spectrometry conference in Minneapolis, MN. Dr. Goebbert also gave invited seminars at Baylor and the University of Georgia. The group has sought outside funding from the National Science Foundation, Army Research Office, and the American Chemical Society Petroleum Research Fund (results still pending). Previous applications submitted during that last academic year included the Department of Energy early career program and the Research Corporation. Dr. Goebbert was

awarded two internal grants – a CASCA proposal for studying the energetics of small cluster ions, and an Arts and Sciences teaching grant to develop new lecture demonstrations. Dr. Goebbert taught CH117 in the fall and implemented more learner-centered techniques and improved assessments. Dr. Goebbert taught physical chemistry lab in the spring, which included five new experiments. Dr. Goebbert served on the Graduate recruiting committee for the department and the student health committee for the university. Dr. Goebbert reviewed multiple manuscripts and proposals.

#### **Dr. Arun Gupta**

- Taught Undergraduate Physical Chemistry II Course (CH 342) in Spring 2014.
- PhD thesis advisor for eight students, including one international exchange students. Two post-doctoral associates in the group.
- Served on several department and university-level committees. Associate Director of the MINT Center. Editorial Board of Nature Scientific Reports and Rare Metals Journals.
- Actively involved in research with 21 refereed articles appearing in print; 4 additional articles accepted or awaiting publication decision; 2 book chapters.
- Total of over 350 refereed journal publications with more than 14,000 citations. H-index of 61.
- Continued research funding through several awards: DOE, NSF- ECCS, NSF-CHE, CRDF, and Industry (Tosyali Properties, LLC).
- Awarded CRSI Medal by the Chemical Research Society of India, February 2014.

**Michael Jennings** - With regards to academic service, Dr. Jennings instructed CH 237 and CH 338 in the fall of 2013. In the spring of 2014, Dr. Jennings instructed CH 232. Based on evaluations (student) for CH 232, CH 237 and CH 338, he received high marks from the undergraduate students. With respect to administrative service, Dr. Jennings has been the Director of Undergraduate Studies since August of 2009. He continues in this role and guides the undergraduate program in chemistry. Dr. Jennings also served as the Chair of the Cava Lecture and Textbook committees. He also serves on the A&S Committee on College Scholarships. With regards to research, the past academic year has been fruitful for his program. His research group (5 graduate students and 3 undergraduates) has synthesized in total (since 2003) twenty-two natural products, (-)-dactylolide, (-)-zampanolide, (-)-varitriol, (-)-centrolobine, (-)-disopongin A, (-)-disopongin B, (+)-bruguierol C, (*epi*)-aigialomycin D, (*rac*)-brussonol, (*rac*)-abrotanone, (-)-clavosolide, (-)-aspergillilde A, (+)-neopeltolide, *ent*-pochonin J, (-)-cyanolide, cryptocarolone, cryptocaryolone diacetate, (7)-desmethoxyfusarentin, sporostatin, xestodecalactone A, curvularin, 12-*oxo*-curvularin, and citreofuran. Dr. Jennings' research group completed the synthesis of three natural products this academic year. In addition to the mentioned natural products, Dr. Jennings' group is investigating the total syntheses of the following natural products: cyanomaclurin, curvulone, zearalenone, neocosmosins B and C, and sinensigenin A. Additionally, Dr. Jennings' research group continues to investigate the catalytic carbocupration of  $\alpha,\beta$ -acetylenic esters with a variety of Grignard reagents for vicinal functionalization protocols. During the past academic 2012-2013 year, Dr. Jennings has given 3 professional presentations and published 3 manuscripts. In addition, Dr. Jennings had continued support via a NSF CAREER award that was completed this academic year. (\$550,000 total over 5 years). As part of his NSF CAREER award, Dr. Jennings hosted a summer research camp for

two rising Bryant High School seniors. These two students carried out research in his lab while also attended the lecture portion of CH 237 during the summer I term. In addition, Dr. Jennings has reviewed numerous manuscripts (>50) for *Organic Letters*, *The Journal of Organic Chemistry*, *The Journal of the American Chemical Society*, *Tetrahedron Letters*, *Pure and Applied Chemistry*, *European Journal of Chemistry*, *The Canadian Journal of Chemistry*, and *Structural Chemistry*. He has also reviewed funding proposals for the American Chemical Society-Petroleum Research Foundation.

**Dr. Diana Leung** - During the Summer 2013, Dr. Leung taught Organic Chemistry I (CH 231, ca. 75 students) and Organic Chemistry Laboratory I (CH 237, ca. 30 students). During the Fall 2013, Dr. Leung taught Introductory Chemistry (CH 104, ca. 340 students) and Organic Chemistry I (CH 231, ca. 200 students). During the Spring 2014, Dr. Leung taught Organic Chemistry Laboratory I (CH 237, ca. 280 students), Organic Chemistry I (CH 231, ca. 210 students), Introductory Organic Chemistry (CH 105, ca. 160 students), Honors Research Seminar (CH 492, 1 student), and Honors Research Seminar (CH494, 3 students). Some of these courses were new preparations, such as CH 104, CH 231, CH 492 and CH 494. In addition, Dr. Leung taught the largest class of CH 237 ever taught at the University in the Spring 2014 (280 students). The courses integrated instructional technology to enhance the students' learning experience, such as extensive use of the Smart Podium, Blackboard Learn, and online homework. Dr. Leung served on the departmental Undergraduate Curriculum Committee, and the College's Diversity Committee with particular involvement in the Capstone Recruitment Days to recruit high school students from Tuscaloosa County and the surrounding Black Belt.

**Dr. Robert Metzger** - The Metzger group continues its work on unimolecular rectification. A major publication (now submitted) took many months of hard editing of a great mass of data. The new and revolutionary project of unimolecular amplification is in the doldrums (trying to make 2 nm thick insulating oxide and nitride films). A major effort to fund all this work failed. A very gifted new student has joined the group, so many new things, including a theoretical thrust, become possible. Never, never, never give up (W. S. Churchill, 1941).

**Dr. David Nikles** - We published three papers, including our first two on our research on polymer waveguides for explosives detection. I took three graduate students and six undergraduates to the spring 2013 National American Chemical Society meeting in New Orleans, April 7 o 11. 2014. We made 12 presentations. Amanda Glover, one of my graduate students, was invited to make an oral presentation in the Symposium on Excellence in Graduate Polymer Research in the Division of Polymer Chemistry. Lindsey Cobb, one of my undergraduates was given a travel grant by the Division of Polymer Chemistry and given an Award for Excellence in Undergraduate Polymer Research. Jerome Arceneaux, a summer REU student from UAB, invited to give a poster presentation at the Conference of Research Experiences for Undergraduates Student Scholarship sponsored by the Council on Undergraduate Research, Arlington, VA, October 27-28, 2013. I was part of a team from A&S, COE and College of Education who won a NSF NUE award to develop a curriculum that introduces the general student population to nanotechnology and its societal, ethical and economic impact. I team taught the first pilot version of this course in the spring semester, 2014.

**Dr. Shanlin Pan** - is finishing his sixth year as an assistant professor. He taught general chemistry in fall and quantitative analysis in spring of the past academic year. Dr. Pan has applied tegrity, clicker and blackboard systems in his class for improving his students' learning outcomes. Dr. Pan supervised 6 graduate students and 6 undergraduate researchers and served on the dissertation committees of 19 students. His current graduate student Mr. **Caleb Hill** received a prestigious Alabama EPSCoR graduate fellowship and also outstanding graduate student of research award this year. Caleb is finishing his PhD degree and will join The Center for Electrochemistry of the University of Texas at Austin as a postdoc to work with the world's famous electrochemist Professor **Allen Bard**. Dr. Pan's former undergraduate student **Karson Brooks** was recently awarded a NSF Graduate Research Fellowship to support her work on polymer chemistry in the University of Georgia. The Pan group recruited additional graduate student Ms. **Nelly Kaneza** whose research interest is to develop self-cleaning SERS electrode materials for molecular sensing and alternative energy conversion. The Pan group has published 6 peer-reviewed journal papers this academic year. He and his students presented 15 presentations at scientific meetings, including 5 invited presentations by Dr. Pan. Professionally, Dr. Pan reviewed 19 journal manuscripts and 24 grant proposals. Together with Auburn, Tuskegee and UAB, Dr. Shanlin Pan developed two new education modules on clean energy and trained middle school teachers to use these modules in their classroom. Along with his collaborators Dr. **Karen Boykin** (UA) and Professor **Dee Goldsten** (UA), Dr. Pan developed and presented his module on light, energy and nanoparticles on MSP NanoBio Science Days of the SECME Summer Institute in Florida. Dr. Pan was involved in the submission of 8 proposals with a total value of nearly \$3 million in the past year. He served as the PI of a pending Major Research Instrument proposal for acquisition of a multichannel pump-probe transient absorption and fluorescence lifetime system for multi-disciplinary research and training at the University of Alabama. Dr. Pan continued serving on the graduate recruiting committee and the diversity committee in this academic year. The group has continued working with Dr. **Arun Gupta** (UA) and his graduate student Ms. **Archana Panikar** on developing surface enhanced technologies for solar photoelectrochemistry reactions. The team has filed a provisional patent with a third-year graduate student Mr. **Zhichao Shan** on his discovery of a nanoelectrode material (NanoCOT) for efficient water splitting. The Pan group has been productive in the area of single molecule spectroscopy under support of the DOE award on interfacial charge transfer in hybrid organic solar cell. Dr. Pan was recently awarded tenure and promoted to associate professor. He was also nominated for the Blavatnik Young Scientist Award by the University and the college A&S Leadership Board Fellowship by the department chair based on his accomplishments.

**Dr. Elizabeth Papish** - Dr. Papish taught Inorganic Chemistry (CH 413/501) in the fall and General Chemistry I (CH 101) in the spring. In CH 413, several new lab experiments were written and test run, and these involved organometallic synthesis and catalysis. At UA, Dr. Papish mentored one post-doctoral fellow, two graduate students and three undergraduate research students this year. During the past year, two Drexel students received the PhD degree and Dr. Papish assisted them remotely in thesis preparation, PhD defense rehearsals, and she travelled to the defense for one student. At UA, she is a member of one additional dissertation committee. Dr. Papish has active funding through an NSF CAREER award that she transferred to UA. She submitted four single investigator proposals this year with a total value of \$1.3 million. Dr. Papish also served as lead PI on a whitepaper submitted to the internal Alabama EPSCOR competition. Dr. Papish had three papers published this year with two papers currently in

progress. She continues to write manuscripts that include Drexel and UA undergraduates and graduate students as co-authors. She also has one patent application pending (for water oxidation and hydrogenation work). She and her students presented one invited and 5 contributed presentations at professional meetings. Dr. Papish also gave seven invited seminars this year. She was a member of the Graduate Committee, Graduate Recruiting Committee, and Materials Science Faculty Search Committee. She devoted significant effort to the department's graduate student recruiting efforts this year. Professionally, she is an active reviewer of manuscripts and proposals and presided at a session at the National ACS meeting.

**Dr. Robin Rogers - Statistics and Highlights for FY14**

- **Personnel:** During FY14, 11 graduate students, 7 undergraduates, 5 postdocs, 2 Research Scientists, and 11 visiting scientists (3 professors, 1 postdoc, 7 international graduate students) were supervised.
- **Award:** Paul Walden Award in Ionic Liquids, Presented by the German Science Foundation Priority Program on Ionic Liquids (SPP 1191)
- **Grants:** 13 new or continuing awards and 15 additional submissions.
- **Papers:** 26 refereed articles and 21 non-refereed abstracts appeared in print; 3 refereed articles are in press and 6 more have been submitted.
- **Meeting Presentations:** 8 total, all invited including 1 Award, 2 Plenary, and 2 Keynote presentations were given at international or national meetings. An additional 18 presentations were given by Group members and collaborators.
- **Seminars:** 10 invited seminars were presented world-wide.
- **Meetings/Symposia Organized:**
  - Chair, *Gordon Research Conference on Ionic Liquids*, Newry, ME, to be held August 17-22, 2014.
  - Theme Organizer “Chemistry and Global Stewardship”, 248<sup>th</sup> ACS National Conference, San Francisco, CA, to be held August 2014.
  - Symposium organizer “Materials Applications of Ionic Liquids (VV)” (with R. E. Del Sesto, S. Dai, and Y. Yoshida) for the 2013 Materials Research Society Spring Meeting (2013), San Francisco, CA.
- **Meeting Advisory Committees:**
  - Advisory Board, 7<sup>th</sup> *Green Solvents Conference*, Dresden, Germany, to be held October 19-22, 2014.
  - International Advisory Board, 6<sup>th</sup> *International Congress on Ionic Liquids (COIL-6)*, Jeju, Korea, to be held June 16-20, 2015.
  - International Advisory Board, Collaborative Conference on Crystal Growth, Phuket, Thailand, to be held Nov. 4-7, 2014.
- **Scientific and Editorial Advisory Boards Served:**
  - Scientific Advisory Board, U.S. Department of Energy Joint Bioenergy Institute, Berkeley, CA, 2010-
  - *Crystal Growth & Design*: Founding Editor-in-Chief, 2000-
  - *Separation Science and Technology*: Editorial Board 1999-
  - *Solvent Extraction and Ion Exchange*, Editorial Board, 2002-
  - *Green Chemistry*, International Advisory Board, 2002-
  - *Chemical Communications*, Editorial Advisory Board, 2005-

- *ChemSusChem*, International Advisory Board, 2008-
- *Chemistry Letters*, Advisory Board, 2010-
- **Guest Editorship:**
- *Green Chemistry and Sustainable Technology*, Springer, Heidelberg, Germany, Book Series Editor (with L.-N. He, D. Su, P. Tundo, and Z. C. Zhang).
- **Intellectual Property:** 6 patents were awarded; 12 patent applications were filed; and two additional invention disclosures were filed with UA. UA executed 2 Non Disclosure Agreements in conjunction with our work.
- **Start-up Companies:** Two start-up companies are being incubated at the Bama Technology Incubator in the AIME building, 525 Solutions, Inc. and IoLiTec Ionic Liquids Technologies Inc. 525 Solutions was awarded a U.S. Department of Energy SBIR Phase I award for “Designing a mini-pilot scale unit for extraction and electrospinning of chitin as an adsorbent for uranium from seawater,” and is currently competing for Phase II funding.

**Dr. Paul Rupar** - Dr. Rupar taught two lecture courses this year, Chemistry 101-001 (268 students) in the first semester and Chemistry 101-003 in the second semester (168 students). Student evaluation of 101-001 was positive and showed improvement from the previous semester. Dr. Rupar currently mentors a group of four graduate students and one undergraduate student and mentored an Emerging Scholar during the Fall 2013 semester. Dr. Rupar participated in numerous professional development programs this year including the David Bauer Grant Writing Seminar. Dr. Rupar served on the Department of Chemistry Graduate Recruitment Committee and serves on the dissertation committee of one graduate student. Dr. submitted two solo-PI proposals, one to the NSF (\$395,322) and one to the Petroleum Research Fund (\$110,000). Dr. Rupar also participated into two joint submissions to the NSF. Dr. Rupar submitted and received an industrial contract with Teknor-Apex worth \$47 760. Dr. Rupar was invited to attend the Cotrell Scholars Collaborative New Faculty Workshop, which helps train new faculty members to be effective scholar-teachers.

**Dr. Kevin Shaughnessy** - The Shaughnessy group research focuses on the application of transition metal catalysts in organic synthetic reactions. The Shaughnessy group had two papers published this year, one of which was selected as a Featured Article by the editors of the *Journal of Organic Chemistry*. Dr. Shaughnessy had two book chapters accepted. In addition to these publications, the Shaughnessy group gave a total of 15 presentations at regional, national, and international meetings and Dr. Shaughnessy presented three invited seminars. Dr. Shaughnessy was PI of a collaborative NSF grant (with Dr. David Dixon) from NSF (\$354,000). He was co-PI (with Dr. Tim Snowden) on an NSF-RUI grant that is subcontracted from Southeastern Louisiana University (\$39,000). New funding was obtained from NSF for a collaborative proposal with Dr. Ryan Hartman in Chemical Engineering (\$352,000), a subcontract of an NSF-SBIR from ThruPore Technologies (\$26,000). He is also co-PI on an NSF-Noyce grant that was awarded to faculty in the College of Education and the Departments of Physics, Chemistry, and Mathematics (\$1.45 million) to increase the number of highly qualified secondary science teachers produced at UA. Dr. Shaughnessy was involved in the submission of 4 proposals during this year with a total value of over \$600K. Dr. Shaughnessy taught two lecture courses this academic year—Organic Chemistry I (CH 231) and Organic Spectroscopy (CH 637) as well as numerous research and independent study courses in line with the standard load for chemistry.

Dr. Shaughnessy generated 732 student credit hours this year. Dr. Shaughnessy continued to receive very high student evaluations of his teaching. Dr. Shaughnessy currently mentors a group of six graduate students and a post-doctoral researcher. Dr. Shaughnessy mentored eight undergraduate research students during 2012-13. Dr. Shaughnessy serves on the dissertation or thesis committee of an additional 24 graduate students. Dr. Shaughnessy serves as Chair of the Department of Chemistry. In addition, his service load included serving on the REU committee, as departmental web master, and as the faculty advisor for Gamma Sigma Epsilon. He also served as an interviewer for the finalists for the University Fellows Experience. Dr. Shaughnessy is a member of the Alabama Science in Motion Steering Committee and serves as the chair of the Awards Committee for the Alabama Section of the ACS. Dr. Shaughnessy reviewed a total of 52 grants and manuscript.

**Dr. Timothy Snowden** - Dr. Snowden mentored four graduate students (Zhexi Li, Jordan Entrekin, Yinghui Liu, and new student Brent Wells), four undergraduate researchers, and a DAAD-sponsored summer intern from Würzburg Germany during the 2013-14 academic year. Dr. Snowden taught CH 231 Organic Chemistry I and AS 101 Chemistry in Everyday Life in the fall and CH 232 Organic Chemistry II in the spring, thereby accounting for 1182 student credit hours. He received high Student Opinions of Instruction scores in all three courses and was nominated for a UA National Alumni Association Outstanding Commitment to Teaching Award. The Snowden group completed two research projects related to new strategies and methods for organic synthesis supported by an NSF CAREER Award. These projects resulted in three publications in 2013-14. As Department Assessment Coordinator, Dr. Snowden devised the 2013-2014 Chemistry Department Assessment Plan that included numerous new assessment measures to document attainment of departmental program goals, and BS degree, MS degree, and PhD degree student learning outcomes. He also prepared the 2012-2013 Chemistry Annual Assessment Report, which outlined many departmental strengths and a few areas needing improvement or further assessment. Dr. Snowden chaired and co-organized the Anthony J. Arduengo, III Lecture in Main Group Element & Physical Organic Chemistry held in April 2014 to honor Professor Hans Reich from the University of Wisconsin. Dr. Snowden also served as a member of the College of Arts & Sciences Tenure and Promotion Committee for a second year and as a member of the Department of Chemistry Graduate Committee. In addition, he reviewed manuscripts for all major scientific publishers, grant proposals for an extramural funding agency, and an organic chemistry textbook for McGraw Hill.

**Dr. Shane Street** - Street Group 13/14The Street group has four papers in near-final form to be submitted. I am or was co-PI on two educational and training grants currently in effect, NSF-REU program, and an Alabama AMSTI training program. I led a collaborative research effort aimed at understanding the interface of dye-sensitized solar cell for a MRSEC preproposal that did not go on to a full proposal this round. I taught two lecture courses in the reporting period, the standard teaching load for the Fall and Spring. In Fall, I taught a Honors General Chemistry (CH 117), to 130 students. In Spring 2014 I taught General Chemistry II (CH 102) with an initial enrollment of 212. I am or was the chair of the dissertation committee for three graduate students (two of them co-advised) and supervise the research of two undergraduates, with the appropriate number of undergraduate research (CH 398) and dissertation research (CH 699) credit hours generated. I serve on the dissertation/thesis committees more than 15 other students. I served on four University committees, and three Departmental committees. I am an A&S

ombudsman, chair of Section A of The University's Research Grants Committee and chair of The University's Laser Safety Committee. I was chair of a faculty search committee for the Department. Other service includes manuscript reviews for seven peer-reviewed journals. I serve on the advisory board of Blackwarrior Riverkeeper. I am the Director of Graduate Recruiting for the Department.

**Dr. Greg Szulczewski** - The Szulczewski group continues to work in the areas of organic spintronics and thermoelectrics. Three manuscripts were published, a book chapter was accepted for publication and two more manuscripts were submitted. The group gave a total of four presentations at international and national meetings. Three proposals were submitted: two at NSF and one to the ACS-Petroleum Research Fund. Dr. Szulczewski gave seminars in the MINT Center and Department of Chemical and Biological Engineering on campus. In addition, he gave an invited talk at the Rodgers Library entitled "Gifts from Nanoscience". In the Fall semester of 2013 Dr. Szulczewski taught CH 524 (Spectroscopic Methods of Analysis); in the Spring semester of 2014 he taught CH 424 (Instrumental Analysis) and CH 102 (General Chemistry). Dr. Szulczewski mentored 3 graduate students (Justin Kreil, Ed Ellingsworth, and Kim Anderson) and 4 undergraduate students (Ali Yousuf, Alexandra Arnold, Lydia Underwood, and Tabatha Sutch) in research. In addition, he served on 18 Ph.D. committees and advised 65 undergraduates. Dr. Szulczewski served on three departmental, one university and one College committee. Dr. Szulczewski reviewed numerous manuscripts for journals including the *Nature Materials*, *Journal of Physical Chemistry*, *Thin Solid Films*, and *Applied Physics Letters*. In addition Dr. Szulczewski reviewed proposals for the Molecular Foundry and National Science Foundation. Dr. Szulczewski served on the 2013 Program Committee of the Magnetic Interfaces and Nanostructures Division of the American Vacuum Society and co-chaired a Symposium on "Gold and silver nanostructures for optical spectroscopy enhancement, sensing and renewable energy" at the April 2013 ACS National Meeting.

**Dr. Russell Timkovich** - A highlight of the year was to put together then teach an upper level special topics course in Nuclear Magnetic Resonance with an emphasis on macromolecular structure determination. The course attracted graduate students specializing in biochemistry, analytical chemistry, and physical chemistry. It began with a thorough examination of NMR fundamentals, then proceeded into NMR instrumentation and techniques with an emphasis on Fourier Transformations and he myriad ways they impact modern NMR technology. Finally, macromolecule structure determination was explored including the use of modern three dimensional experiments and how to interpret them. Course assignments included hands-on lab work on advanced experiments. On the research front, work is continuing on the full assignment of all protons, carbons, and nitrogens in the catalytic domain of zoocin A designated C74A. This is a necessary first step toward determining experimental restraints that will ultimately lead to a structure for C74A.

**Dr. Thomas Vaid** - Prof. Vaid was the coauthor of two published papers, "Electronic Structure and Photophysics of (C=C)tetra-*p*-tolylporphyrin<sup>2+</sup>", in *Photochem. Photobiol. Sci.* and "Computational Screening of Structural and Compositional Factors for Electrically Conductive Coordination Polymers", in *Phys. Chem. Chem. Phys.* A third manuscript, "3D Printed Molecules and Extended Solid Models for Teaching Symmetry and Point Groups", completed in collaboration with science librarian Vincent Scalfani, was accepted for publication in *J. Chem.*



*Educ.* A story concerning that publication will appear in the May 19 issue of *Chemical and Engineering News*. Prof. Vaid gave two talks concerning his research in the past year, a contributed talk at the Spring ACS National Meeting in New Orleans, and an invited talk at SERMACS in Atlanta.

**Dr. John Vincent** – Prof. Vincent gave invited talks at the international, national and local level while the Vincent group additionally gave three presentations at national meetings and one presentation at a regional meeting. Prof. Vincent had one book, one peer-reviewed article, one peer-reviewed letter, three encyclopedia entries, and one book chapter published and had one peer-reviewed article accepted for publication. Prof. Vincent had continuing funding from NSF and AICHE and new funding from AICHE. Research in the group is focused on 1) characterizing the chromium biomolecule low-molecular-weight chromium-binding substance (LMWCr or chromodulin) found in body tissues and lost from the body in urine and 2) examining the mechanism by which chromium can have pharmacological effects increasing insulin sensitivity and improving cholesterol levels. Prof. Vincent serves as Co-chair of the Faculty Senate's Academic Affairs Committee. Prof. Vincent served on three University Standing Committees including being vice-chair of the IACUC and chair of the laboratory safety committee and on numerous other University committees. Prof. Vincent served on the editorial board of two journals, on the State of Alabama Radiation Advisory Board of Health, and on the Chemistry Committee of the State of Alabama Articulation and General Studies Committee. In an April 23, 2014 review of citations on ISI Web of Science, Dr. Vincent had 124 publications identified (excluding abstracts, letters, corrections, etc.) that resulted in 7,321 citations, giving an average of 59 citations per publication. He has an H-index of 43. Dr. Vincent has one publication cited over 1300 times.

**Stephen Woski** - The research program of Prof. Woski has continued to progress in several directions. In the research area of molecular electronics, work expanded on the applications of hemibiquinones as rectifying modules. Work is underway to append functional groups that will allow for self-assembled monolayer formation on electrode surfaces. Profs. Woski and Street continue a collaborative project to develop new molecules to simultaneously bind sensitizing dyes to semiconductor surfaces while protecting these fragile moieties by surrounding them in lipid-like groups. Studies of the chemistry of nucleic acids containing modified nucleoside residues have also continued. Two manuscripts from this work are in preparation. In service, Woski continues to serve as the Department of Chemistry's Director of Graduate Studies. One of the major requirements in the graduate program (the literature seminar) has been substituted by a course "Literature & Communication in Graduate Chemistry". This course was co-taught with faculty from the UA Libraries in Fall 2013 and will be offered again in 2014. In December, a faculty retreat was held to discuss the structure of our graduate program and what could be done to better prepare our students while maintaining the goal of minimizing the time to degree. Changes to the candidacy exams, the schedule of student/committee meetings, and the first year courses are under consideration. Woski served as co-PI and co-director (with Blackstock) of the final year of our GAANN program to enhance graduate education from the Dept of Education. Woski was co-PI on a funded proposal to the NSF (Research Experiences for Undergraduates in Chemistry at the University of Alabama). This project provides 10-week research experiences for undergraduates interested in a career in chemistry. Students are primarily chosen from

smaller institutions around the Southeast that cannot provide similar opportunities for research. This grant has recently been renewed.

## **II. Staff Highlights**

**Staff Awards:** Ms. April McIntosh received the Office, Clerical, and Technical Staff Associate Outstanding Staff Award. Ms. McIntosh is a senior office associate for the Department's endowed chair faculty. Mr. Richard Smith was nominated for the Outstanding Professional Staff Award presented by the Professional Staff Association.

**Staff Changes:** Ms. Carolyn Walker retired after a long career serving the department as accounting specialist. Ms. Reda Arnold was promoted to the accounting specialist position. Ms. Amy Francko was hired as an office associate in the business office to replace Ms. Arnold. Mr. Bradley Smith was hired as a materials clerk to assist in the Shelby Hall stockroom.

## **III. Student Highlights**

Department students received recognition on campus and nationally for their academic and research success. Major awards are highlighted here, while the complete list of awards received by department graduate and undergraduate students is provided below.

### **Graduate Student Fellowships and Awards**

#### **External Awards**

##### **ACHE Graduate Research Scholars Fellowship**

Caleb M. Hill (Pan)

##### **NSF Graduate Research Fellow**

Jordyn L. Johnson (Frantom)

##### **Nuclear Energy University Program Fellowship**

Steven P. Kelley (Rogers)

##### **National Defense Science & Engineering Graduate Fellowship**

Parker D. McCrary (Rogers)

##### **Southern Regional Education Board Fellowship**

Melody D. Kelley (Blackstock)

##### **Howard Hughes Medical Institute Fellowship**

Michelle L. Stover (Dixon)

##### **The Annual School on X-Ray & Neutron Scattering Meeting**

Steven P. Kelly (Rogers)

##### **63<sup>rd</sup> Lindau Nobel Laureate Meeting**

Steven P. Kelley (Rogers)      Michele L, Stover (Dixon)

## **University Awards**

### **Graduate Council Fellowship**

C. J. Pruitt (Goebbert)

### **National Alumni Association License Tag Fellowships**

Jordan T. Entrekin (Snowden)

### **McNair Graduate Fellowship**

Pandora E. White (Vincent)

### **3-Minute Thesis Competition**

Steven P. Kelley (Rogers)—2<sup>nd</sup> place in University-wide competition

## **A&S Awards**

### **A&S Outstanding Dissertation Award**

Mier An (Busenlehner)

### **A&S Outstanding Dissertation Research Award**

Mingyang Chen (Dixon)

### **Dean's Diversity Scholarship**

Pandora E. White (Vincent)

## **Chemistry Department Awards**

### **Outstanding Graduate Student Award**

Caleb Hill (Pan)                      Parker McCrary (Rogers)

### **Outstanding Third-Year Student Award**

Archana Panikar (Gupta)

### **Outstanding Second-Year Student Award**

Ian Adams (Rupar)

### **Outstanding First-Year Teaching Award**

Rachael Albury (Goebbert)

### **3-Minute Thesis Competition**

Steven P. Kelley (Rogers)                      Joseph E. Meany (Woski)  
Gregory W. Dye (Street)                      Leah E. Block (Rogers)

## **Undergraduate Student Awards**

### **External Awards**

#### **Biotechnology Internship at HudsonAlpha Institute**

Anna E. Willis

**Student Representative to UN Climate Change Conference**

Emily R. Bloomquist

**Accompanying Jr. Researcher on the Alexander von Humboldt**

Wesley F. Taylor (Arduengo)

**University Awards**

**Randall Outstanding Undergraduate Research Awards**

Ronneshia Jackson

Meredith Rickard (Dixon)

Morgan E. Whitaker (Nikles)

Shuwen Yue (Dixon)

**H. Pettus Randall, Jr. Scholarship**

Meredith M. Rickard (Dixon)

**The Catherine Johnson Randall Award**

Joshua D. Moon (Dixon)

**Phi Beta Kappa**

Margaret G. Apperson

Stephen A. Walker

Travis J. Atchley

Anna E. Willis

Garrett H. Taylor

Kristi Y. Wu

**Undergraduate Research and Creative Activity Conference**

2<sup>nd</sup> Place Oral: Megan Johnston (Shaughnessy)

4<sup>th</sup> Place Oral: Shuwen Yue (Dixon)

Honorable Mention Oral: Travis Atchley (Blackstock)

1<sup>st</sup> Place Poster: Morgan Whitaker (Nikles)

3<sup>rd</sup> Place Poster: Sarah McFann

Honorable Mention Poster: Amanda Volke (Nikles)

1<sup>st</sup> Place, Emerging Scholars Oral: Erin Hein (Busenlehner)

**A&S Awards**

**Dean's Award of Merit**

Ronneshia L. Jackson

Garrett H. Taylor

**Distinguished Undergraduate Scholars**

Margaret Pringle Johnson

Eric J. Wenzinger

**2014 Outstanding Senior Award Recipients**

Mary Katherine Sweeney

Garrett H. Taylor

**Michael T. Wilder Memorial Endowed Scholarship**

Olivia C. Roe

## **Chemistry Department Awards**

### **Outstanding Chemistry Undergraduate Student Award**

Jesse Gettinger

### **Outstanding Chemistry Undergraduate Student Research Award**

Morgan Whitaker

### **The American Institute of Chemists Award**

Evan McConnell

### **ACS Division of Inorganic Chemistry Undergraduate Student Award**

Eric Wenzinger

### **ACS Division of Organic Chemistry Undergraduate Student Award**

Travis Atchley

### **Outstanding Analytical Chemistry Student Award**

Sean Miller

### **Outstanding Organic Chemistry Students Award**

Garrett Diltz

Kelli Reese

Kindle Williams

### **Outstanding Nursing Student Award**

Catherine Roveda

### **Outstanding General Chemistry Students Award**

Adam N. Bonertz

Justin W. Magrath

Travis A. Upton

Alexander J. Franz

Jacob R. Mellon

Michelle B. Weyhaupt

Jacqueline R. Harris

Michael M. Royko

Kayleigh A. Yackels

Amanda K. Ivy

Haley E. Taylor

### **2012 Alabama Chapter of Gamma Sigma Epsilon National Chemistry Honorary Society**

Cameran Beg

Thomas Ludwig

Haley Burhans

Max Mittenthal

Elizabeth Cook

Lisa Marie Morgan

Katherine Donaldson

Julia Murphy

Sarah Fleisher

Joseph Neff

Sawyer Foyle

Jocelyn Newman

Christopher Griffith

Jacob Owen

Ryan Hacherl

Shanna Phillips

Lauren Hagler

Meredith Rickard

Erin Hein  
Rachel Honan  
Katlyn Hughes  
Elle Kaplan

Mallory Smith  
Samantha Tilson  
James Vegrzyn  
Kindle Williams

#### IV. Faculty Research Productivity

**Publications and Presentations:** The Chemistry faculty had a highly productive year in terms of research publication of research and presentation of their research results at meetings and in invited seminars (Tables 1 and 2). The chemistry faculty published 128 peer-reviewed papers during this year, which is the highest total over the past five years. This corresponds to 4.9 publications per faculty member. Another 11 papers have been accepted, but had not been published as of March 31, 2014. The faculty submitted a total of 125 papers (4.8/faculty) during this FAR year, which includes some of the papers that were also published in 2013-14. A total of 22 patent applications were submitted this year and 7 patents were awarded to Department faculty. The faculty were highly active in presenting their research with a total of 232 presentations at professional meetings and invited seminars at other schools.

**Table 1. Summary of Faculty Research Productivity by Year**

Year	Published Articles <sup>a</sup>	C&G awarded (\$)	C&G sub <sup>b</sup> (\$)	C&G In-Force	Research Exp. <sup>c</sup>	Talks
2013-14	128	22 (\$3.8 M)	104 (\$22 M)	72 (\$13.6 M)	\$3.33 M	232
2012-13	115	17 (\$2.2 M)	100 (\$21 M)	79 (\$13.8 M)	\$3.73 M	169
2011-12	102	47 (\$3.8 M)	92 (\$23 M)	52 (\$11.2 M)	\$4.00 M	210
2010-11	123	34 (\$2.9 M)	109 (\$32 M)	65 (\$15.2 M)	\$3.40 M	197
2009-10	91	47 (\$5.6 M)	163 (\$55 M)	45 (\$11.5 M)	\$3.22 M	138

<sup>a</sup>Peer-reviewed articles published in this FAR period. <sup>b</sup>Submitted proposal applications that are pending or were not funded. <sup>c</sup>Fiscal year (10/1–9/31) research expenditures (2013-14 value is FY 13) from OSP annual report.

**Contract and Grant Activity:** The Department faculty had a strong year of contract and grant activity (Tables 1 and 3). Chemistry faculty submitted 104 proposals (84 proposal equivalents) with a total value of \$22 million, which is an increase of \$1 million over 2012-13. Faculty were awarded 22 contracts and grants (18 proposal equivalents) with a value of \$3.8 million, which is a significant improvement in both number of awards and awarded dollars from last year. The number of in-force awards is down from last year, but still above the previous 3 years. The dollar amount of in-force funding, \$13.6 million, is \$200K lower than in 2012-2013. Combining new awards and in-force dollars shows that the total active research funding for this year is higher than last year. Research expenditures were down in FY 13 from the prior two years, but should be expected to rise with the increase in grant funding this year. The significant increase in new funding is a positive sign, particularly in this difficult funding climate. It is also gratifying to see the continued high level of submission activity by the faculty given the fact that many federal and private agencies are limiting the number of submissions that an individual PI can make in a given year.

**Table 2. Individual Faculty Publication Activity<sup>a</sup>**

Faculty	Peer-Reviewed Publications			Books		Patents		Talks
	Sub	Acc	Pub	Book	Chap	App	Iss	
Arduengo	6	0	7	0	1	0	0	10
Bakker	4	0	4	0	0	2	1	5
Blackstock	0	0	0	0	0	1	0	8
Bonizzoni	4	1	3	0	0	0	0	17
Bowman	4	0	7	0	0	0	0	11
Busenlehner	3	0	2	0	1	0	0	11
Cassady	0	0	1	0	0	1	0	0
Dixon	24	2	28	0	1	0	0	23
Frantom	3	1	1	0	0	0	0	11
Goebbert	4	1	4	0	0	0	0	4
Gupta	16	1	21	0	2	1	0	14
Jennings	3	0	3	0	0	0	0	3
Metzger	0	0	1	0	1	0	0	2
Nikles	3	0	3	0	0	0	0	16
Pan	5	0	6	0	0	2	0	27
Papish	2	0	3	0	0	1	0	13
Rogers	28	4	22	0	3	12	6	17
Rupar	0	0	0	0	0	0	0	3
Shaughnessy	2	0	2	0	3	1	0	20
Snowden	3	0	3	0	0	0	0	2
Street	0	0	0	0	0	0	0	1
Szulczewski	5	0	2	0	0	0	0	4
Timkovich	2	0	2	0	0	0	0	0
Vaid	3	1	2	0	0	0	0	2
Vincent	1	0	1	1	1	1	0	7
Woski	0	0	0	0	0	0	0	1
<b>Total</b>	<b>125</b>	<b>11</b>	<b>128</b>	<b>1</b>	<b>13</b>	<b>22</b>	<b>7</b>	<b>232</b>

<sup>a</sup>Accepted publications are those that have been accepted, but not published. Publication submissions (sub) include all peer-reviewed papers submitted this year, including those also accepted or published.

**Table 3. Individual Faculty Grant Activity<sup>a</sup>**

Faculty	Submitted	Submitted \$	Awarded	Awarded \$	In-Force	In-Force \$
Arduengo	10	\$1,360,502	2	\$7,405	1	\$90,000
Bakker	3	\$212,500	2	\$13,682	4	\$193,361
Blackstock	0	\$0	0	0	3	\$289,092
Bonizzoni	3	\$1,571,677	0	0	2	\$8,997
Bowman	1	\$371,530	1	\$66,874	1	\$199,793
Busenlehner	3	\$2,045,142	0	0	1	\$697,501
Cassady	1	\$130,512	2	\$575,830	3	\$339,464
Dixon	9	\$3,533,292	3	\$874,521	13	\$4,228,813
Frantom	2	\$283,104	0	0	2	\$659,527
Goebbert	6	\$1,972,023	2	\$3,100	1	\$6,000
Gupta	8	\$2,291,876	1	\$88,090	6	\$1,547,792
Jennings	1	\$490,858	0	0	1	\$550,000
Metzger	1	\$522,326	0	0	1	\$365,000
Nikles	3	\$446,095	0	0	1	\$34,000
Pan	8	\$2,942,305	0	0	4	\$1,017,375
Papish	4	\$1,311,705	1	\$140,901	0	0
Rogers	17	\$4,654,609	2	\$1,121,591	13	\$1,488,614
Rupar	6	\$921,614	1	\$47,760	0	0
Shaughnessy	4	\$639,700	2	\$316,482	3	\$390,034
Snowden	1	\$5,500	1	\$5,500	2	\$589,119
Street	3	\$287,411	1	\$11,000	2	\$65,741
Szulczewski	2	\$183,168	0	0	1	\$5,000
Timkovich	1	\$183,182	0	0	0	0
Vaid	3	\$522,654	0	0	0	0
Vincent	3	\$1,336,031	1	\$9,996	4	\$181,861
Woski	1	\$191,141	0	0	3	\$681,291
<b>Total</b>	<b>104</b>	<b>\$28,410,457</b>	<b>22</b>	<b>\$3,282,732</b>	<b>72</b>	<b>\$13,628,375</b>

<sup>a</sup>In-force C&G refer to grants in force on 3/31/13. Awarded includes grants funded in this period, while submissions includes all grants submitted in this period, including those funded, pending, or declined.

## V. Credit Hour Production and Numbers of Majors/Graduates

### Student Credit Hour Production

The total student credit hour production (graduate and undergraduate) was 15,050 and 11,698 in the fall 2013 and spring 2014 semesters, respectively. The total of 26,748 SCH represents a 10% increase compared to 2012-13, which continues a six year string of double digit percentage growth in credit hour production. Table 4 shows the past five years of enrollment trends in Chemistry. The Department has seen a 63% increase in credit hour production from 2009-10 to 2013-14. The bulk of this growth has been at the undergraduate level, primarily in the service level courses. Student credit hours have grown 69% at the undergraduate level and 37% at the graduate over the past five years.



**Table 4. Total Credit Hour production**

Academic Year	Undergraduate	Graduate	Total	% Change
2013-2014	25,165	1,583	26,748	+13%
2012-2013	22,207	1,528	23,735	+18%
2011-2012	18,747	1,395	20,142	+10%
2010-2011	16,901	1,373	18,274	+14%
2009-2010	14,847	1,155	16,002	+10%

The Department continues to see significant growth across the undergraduate curriculum. Total credit hour production by semester for undergraduate courses is shown in Table 5, and Table 6 shows a breakdown by course level. The 100-level courses and organic chemistry represent the Department's main service teaching load. The Department continues to see significant growth in our service courses. The 100 level courses (101/102, 104/105, and 117/118) grew by 9% over last year and have grown by approximately 69% since 2009-10. Organic chemistry showed significant growth this year of 31%, which reflects the greater than 30% growth seen in general chemistry (CH 101/102/117/118) in 2012-13. A smaller growth should be expected for next year, based on the relatively small growth at the 100 level this year. Student credit hour production in the upper level chemistry courses (300-400 level) increased significantly (23%) for the second straight year. This increase reflects the recent growth in the number of chemistry majors, who are main audience for our 300- and 400-level courses. In addition, our biochemistry course (CH 461) is a popular course for biology majors and chemical engineering majors.

**Table 5. Overall Trends in Undergraduate Credit Hour Production.**

Academic Year	Fall Semester	Spring Semester	Total (% growth)
2013-2014	14,210	10,955	25,165 (13%)
2012-2013	12,090	10,117	22,207 (18%)
2011-2012	10,287	8,460	18,747 (11%)
2010-2011	9,166	7,735	16,901 (14%)
2009-2010	8,165	6,682	14,847 (8%)

**Table 6. Credit Hour Production by Course Level**

Academic Year	100 Level	Organic	Upper (% growth)
2013-2014	18,824 (9%)	5,035 (31%)	1306 (23%)
2012-2013	17,288 (22%)	3,855 (6%)	1,064 (20%)
2011-2012	14,222 (9%)	3,642 (22%)	883 (1%)
2010-2011	13,052 (17%)	2,974 (9%)	875 (-12%)
2009-2010	11,132 (9%)	2,721 (3%)	994 (11%)

Graduate student credit hour production grew by 4% over 2012-13, which continues a six year trend of strong growth in graduate SCHs as our graduate population has increased. Student credit hours have increased by 37% since 2009-10.

**Table 7. Trends in Graduate Credit Hour Production**

Academic Year	Fall Semester	Spring Semester	Total
2013-2014	840	743	1,583 (4%)
2012-2013	796	732	1,528 (10%)
2011-2012	637	758	1,395 (2%)
2010-2011	684	689	1,373 (19%)
2009-2010	587	568	1,155 (41%)

**Table 8. Credit Hour Production by Tenure/Tenure-Track Faculty Members**

Faculty	Fall 2013			Spring 2014			Total SCH
	UG SCH	G SCH	Total	UG SCH	G SCH	Total	
Arduengo	6	11	17	12	15	27	44
Bakker	4	13	17	780	13	793	810
Blackstock	3	59	62	361	24	385	447
Bonizzoni	349	15	364	4	29	33	397
Bowman	90	19	109	780	23	803	912
Busenlehner	765	20	785	60	12	72	857
Cassady	180	18	198	0	48	48	246
Dixon	73	34	107	2	21	23	130
Frantom	209	118	327	0	27	27	354
Goebbert	246	20	266	31	22	53	319
Gupta	0	16	16	51	18	69	85
Jennings	347	16	363	472	18	490	853
Metzger	0	145	145	0	167	167	312
Nikles	744	10	754	853	10	863	1,617
Pan	756	24	780	190	26	216	996
Papish	55	50	105	818	7	825	930
Rogers	587	47	634	1	40	41	675
Rupar	1,075	6	1,081	675	15	690	1,771
Shaughnessy	647	19	666	11	55	66	732
Snowden	662	25	687	468	27	495	1,182
Street	521	18	539	853	13	866	1,405
Szulczewski	1	61	62	709	10	719	781
Timkovich	564	6	570	0	24	24	594
Vaid	1,036	6	1,042	6	14	20	1,062
Vincent	766	13	779	283	15	298	1,077
Woski	10	46	56	102	56	158	214
Total	9,696	835	10,531	7,522	749	8,271	18,802
Average	373	32	405	289	29	318	723
Median	347	19	363	60	21	167	781

Student credit hour values include both lecture courses and independent study courses at the graduate and undergraduate level taught by each faculty.

The Chemistry faculty have remained highly productive in student credit hour production per tenured/tenure-track (TT) faculty. Table 8 shows the credit hour production by each TT faculty

member for the 2013-14 academic year. For the fall semester, Chemistry TT faculty averaged 373 SCH (median 347). For the academic year, the departmental average was 723 student credit hours per faculty over the two-semester period while the median production was 781 SCH. It is anticipated that the SCH production/faculty member will remain high next year with further growth in our service classes.

The Department's reliance on non-tenure track faculty to meet its instructional needs remains high (Table 9). As a CLTF, Dr. Diana Leung generated over 3,000 SCH this year. In addition, a total of 8 PTTI lines were used during the academic year. Part-time instructors generated nearly 5,000 SCH in the department this year. After decreasing our reliance on PTTI lines during the 2012-13 academic year, continued student growth resulted in an increase in the number of PTTI lines required.

**Table 9. Credit Hour Production by Non-Tenure Track Faculty**

<b>Faculty</b>	<b>Rank</b>	<b>Fall SCH</b>	<b>Spring SCH</b>	<b>Total SCH</b>
Leung	CLTF	1,906	1,186	3,092
Barber	PTTI (1 class)	748	0	748
McDuffie	PTTI (3 classes)	564	798	1,362
Scheiner	PTTI (4 classes)	1,316	1,540	2,856
<b>Total</b>		<b>4,534</b>	<b>3,524</b>	<b>8,058</b>

### **Undergraduate Majors and BS Degrees**

The number of students declaring chemistry as their major in the spring semester of 2014 was 206, up 49% from the spring of 2012 (Table 10). The number of majors in Chemistry has grown over the past two years after several years of little change in the number of majors. The Department has made a concerted effort to grow our majors as the overall university population grows. The Chemistry Department continues its effort in attracting and retaining chemistry majors to continue to build on these trends. Increased enrollment in 200- and 300-level courses taken solely by Chemistry majors shows that this growth is occurring at all levels, but is focused in the 1<sup>st</sup> and 2<sup>nd</sup> years of the curriculum. Growth in the number of chemistry graduates is anticipated in coming years, after having smaller classes over the past few years.

**Table 10. Undergraduate Chemistry Major Trends**

<b>Year</b>	<b>Fall</b>	<b>Spring</b>
<b>2013-14</b>	192	206
<b>2012-13</b>	156	181
<b>2011-12</b>	157	138
<b>2010-11</b>	144	119
<b>2009-10</b>	140	128

During the calendar year of 2013, the Chemistry Department graduated 20 students (Table 11). This represents a slight increase over the 2012 calendar year. Of particular note, half of the graduates earned the more rigorous ACS-certified degree, plus one student who graduated on the Chemical Engineering/Chemistry dual degree track. Three fourths of our graduates (15/20) graduated with distinction (*cum laude* or higher). We can anticipate a significant increase in graduates next year as 26 students graduated with Chemistry degrees in May, which is the largest May class in the past six years. Given the Department's growth in majors and enrollment in

upper level courses, growth in Chemistry degree production should continue for the next several years.

**Table 11. Undergraduate Degree Production**

<b>Year</b>	<b>Degree</b>	<b>May</b>	<b>Aug</b>	<b>Dec</b>	<b>Total</b>
<b>2013</b>	Pre-Health	7	1	1	9
	ChE/CH	0	1	0	1
	ACS	9	0	1	10
	<b>Total</b>	<b>16</b>	<b>2</b>	<b>2</b>	<b>20</b>
<b>2012</b>	Pre-Health	6	2	0	8
	ACS	9	1	0	10
	<b>Total</b>	<b>15</b>	<b>3</b>	<b>0</b>	<b>18</b>
<b>2011</b>	Pre-Health	11	0	1	12
	ACS	10	0	1	11
	<b>Total</b>	<b>21</b>	<b>0</b>	<b>2</b>	<b>23</b>
<b>2010</b>	Pre-Health	11	1	1	13
	ACS	10	0	3	13
	<b>Total</b>	<b>21</b>	<b>1</b>	<b>4</b>	<b>26</b>
<b>2009</b>	Pre-Health	8	0	1	7
	CH/BCH	8	0	1	11
	ACS	2	1	0	3
	<b>Total</b>	<b>18</b>	<b>1</b>	<b>2</b>	<b>21</b>

#### **Undergraduate Curriculum Changes and Projects**

Dr. Shaughnessy is co-PI on an NSF NOYCE grant that seeks increase the number of physical science (chemistry and physics) and math students pursuing secondary education certification from UA. As part of this effort, Dr. Shaughnessy is exploring potential new certification pathways for highly qualified teachers with chemistry training. Dr. David Dixon is co-PI on an HHMI grant that is supporting curricular improvements in the Honors Chemistry lab courses.

#### **Graduate Student Population and Degree Production**

Some Graduate Program vital statistics for April 1, 2013 to March 31, 2014 compared to previous years are given below in Tables 12-16. Graduate enrollment in fall 2013 increased slightly to 97 doctoral+masters students, which is an average of 3.7 students/tenured or tenure-track faculty. Enrollment of students from underrepresented groups continued to be strong with women comprising 40% and African-Americans/Hispanics/Native-Americans comprising 21.5% of domestic graduate student population. The graduate student population continues to hold with clear majority of domestic students versus international students (67% vs. 33%). Of note, we have now successfully recruited 5 international students from Africa. These students have attended US undergraduate programs and possess excellent English skills, marking this cadre as a potential future source of high quality graduate students.

**Table 12. Graduate Student Enrollment Trends**

Year	Total Students	Ph.D.	M.S.	PLA (Ph.D.)	Postdocs
<b>Fall 2013</b>	<b>97</b>	<b>95</b>	<b>2</b>	<b>0</b>	<b>15</b>
Fall 2012	94	93	1	0	12
Fall 2011	94	93	0	1	13
Fall 2010	83	82	0	1	16
Fall 2009	77	77	0	0	6

**Table 13. Domestic/Foreign Student Distribution.**

Year	USA	Foreign
<b>Fall 2013</b>	<b>65</b>	<b>32</b>
Fall 2012	65	29
Fall 2011	66	27
Fall 2010	61	22
Fall 2009	49	28

**Table 14. Nationality Distribution.**

Year	USA	China	India	Eastern Europe	Other South/East Asia	Other
<b>Fall 2013</b>	<b>65</b>	<b>19</b>	<b>4</b>	<b>1</b>	<b>2</b>	<b>6</b>
Fall 2012	65	17	7	1	1	3
Fall 2011	66	16	8	1	0	2
Fall 2010	61	13	6	2	1	0
Fall 2009	49	14	5	5	2	2

**Table 15. Gender and Minority Distribution.**

Year	Total	Male	Female
<b>Fall 13</b>	<b>97</b>	<b>58</b>	<b>39</b>
Fall 12	94	56	38
Fall 11	94	55	39
Fall 10	83	47	36
Fall 09	77	42	35

**Table 16 Domestic Gender and Minority Distribution.**

Year	Male	Female	African-American	Hispanic	Native-American
<b>Fall 13</b>	<b>37</b>	<b>28</b>	<b>11</b>	<b>1</b>	<b>1</b>
Fall 12	39	26	10	1	1
Fall 11	39	27	11	0	1
Fall 10	36	26	10	1	0
Fall 09	29	20	7	1	0

A snapshot of the methods of supporting our graduate student population for fall 2014 is shown in Table 17. The number of TAs allotted to fulfill our teaching mission has increased to 55.4 TAs for AY 2013-14, 11 of which are soft money TAs. We purposefully oversubscribed by 5 TA lines in Fall 2013. This overage was partly recovered in spring 2014 when we employed 51.0 TAs. We expect the budget to balance with the summer appointments. With enrollment increases projected to continue, the recent “hardening” of TA lines to reach 50.4 and addition of 9 soft TA lines will hopefully meet our Fall 2014 needs. We expect that we will be oversubscribed again this fall as we are aggressively recruiting new students and have several students finishing their dissertations.

Additionally, the Department would ultimately like to reduce the lab teaching load of TAs from 3 general chemistry lab sections per semester to 2 lab sections, while adding recitation sessions to the TA duties (see Department needs). These recitation sections will provide students in large lecture classes an opportunity to meet in a smaller group setting where they can actively participate in problem solving exercises. Doing so will enhance student success and improve retention in the lower level courses, as well as improving graduate student learning outcomes.

The number of students on RA support dropped compared to the previous fall (Table 17). Faculty need to continue to strive to provide RA support for graduate students in order to grow the overall graduate population significantly. The Department aspires to a ratio of RA:TA lines of >1, which we have not met since fall 2007. This ratio was difficult to maintain due to the dramatic increase in TA lines prompted by the growth of the University. However, the challenging current funding climate is also reflected in the drop in funded RAs in the current year.

University-sponsored graduate fellowships are critical funding resources for the program. Fellowships and scholarships funded for AY 2013-14 are shown below, along with those from several previous years. For this academic year, the chemistry department had 3 students on 9-month fellowships awarded by the graduate school. In addition, Chemistry students received fellowship support from a number of external sources including NSF, DOE, DOD, and the US Army. The end of the GAANN funding was responsible for the decrease in external fellowships in the current year. We intend to reapply for this grant when/if the program is restarted.

**Table 17. Methods Used to Support the Graduate Students.**

Year	TA	RA	Staff	External Fellowship	Internal Fellowship	Department	Self Support
<b>Fall 13</b>	<b>60.50</b>	<b>22.16</b>	<b>0</b>	<b>6</b>	<b>3</b>	<b>0</b>	<b>6</b>
Fall 12	47.00	27.66	0	13	4	0	5
Fall 11	45.66	27.33	0	11	3	0	8
Fall 10	40.83	25.83	0	10	5	0	3
Fall 09	37.66	29.33	0	3	5	0	4
Fall 08	36.00	24.33	0	6	4	0	4
Fall 07	30.33	34.33	0	2	3	0	5
Fall 06	28.33	36.66	1	4		0	2

**Support breakdown: TAs:** 60.50 = 16.33 first-year students, 11.00 second-year students, 33.16 third-year and beyond. **RAs:** 22.16 = 1.00 first-year student, 1.00 second-year student, 20.16 third-year and beyond. **Fellowships:** 1 GCF (C. Pruitt), 1 NAA (J. Entrekkin), McNair (P. White), 1 NSF (J. Johnson), 1 SREB (M. Kelley), 1 DOE/NEUP (S. Kelly), 1 DOD (P. McCrary), 1 ACHE (D. Clayton), 1 US Army (C. Griggs).

A total of 18 students received graduate degrees from the department last year (10 MS and 8 PhD). It is anticipated that the number of doctoral graduates will increase in the coming year.

**Table 18. Graduate Degree Production Trends.**

<b>Calendar Year</b>	<b>MS</b>	<b>PhD</b>	<b>Total</b>
<b>2013</b>	<b>10</b>	<b>10</b>	<b>20</b>
2012	10	8	18
2011	7	7	14
2010	9	9	18
2009	4	12	16
2008	7	13	20
2007	6	15	21
2006	1	11	12

**Table 19. 2013-2014 PhD degrees**

<b>December 2013</b>	<b>Spring 2014</b>	<b>Summer 2014 (anticipated)</b>
Amy Grano	Dripta DeJoarder	Edward Garner
Virgil Jackson	Zongtang Fang	Leslie Gentry
Justin Kreil	Sharifa Love	Melody Kelley
Harsimran Singh	Parker McCrary	Jane Moore
Xueyu Zhang	Yu Wang	

### **Graduate Student Recruiting and Admissions**

A total of seventeen (17) students entered our graduate program in AY 13/14. This class was supported by 17 full or partial graduate teaching assistantships (TAs), one fellowship, and two partial RAs. This class included seven females and ten males. Eight of these students were US citizens and nine were foreign nationals.

A fall 2014 incoming class of fifteen students is currently committed, with perhaps just a few more possible, depending on funding. The entering class (as is) will be supported by twelve full or partial TAs, and partially supported by two Graduate Council Fellowships with departmental enhancements, one Kuwaiti Scholar, and two UA University Scholars in the MS program.

Our graduate TA stipend (also usual for RAs) of \$23,232, with no-cost health coverage, for AY 2013-14 is competitive with schools in the Southeast as determined from the recent SE Chair's Survey. Net regional stipends range from \$18,000-27,000. Our stipend will likely need to be increased in the near future, especially as fees (such as credit hour fees) begin to degrade the value of our stipends. Keeping a competitive stipend is critical to student recruiting. It should be noted that to attract some of the best students we (along with the Graduate School and Dean's office) have been able to make a very few offers with stipends nearing \$30,000/yr. (e.g., Graduate Council Fellowships with departmental enhancements, coupled with partial TA and possibly other awards). Nevertheless, not all such offers are accepted given the very stiff competition for these students.

**Tables 20-23** show pertinent data on graduate admissions. The quality of our incoming students remains good overall, but there is a real distinction between high quality students

admitted under fellowships and selected for initial rounds of offers and the rest of the admitted class. The fifteen students admitted for fall 2014 have an average GRE score of 308, and three are conditional admission. One student received a Dean's Diversity award accepted our admissions offer. Five of our nominated students were awarded Graduate Council Fellowships, and two of these accepted.

**Table 20. Incoming Students – Number and Type of Admissions and Average Test Scores.**

	Total	Regular	Conditional	PLA	Domestic	Foreign	Avg. GRE	Avg. TOEFL
F 14*	15	11	3	1	11	4	308	
Sp 14	1	1	0	0	1	0	313	
F 14	18	11	5	0	10	8	306	92 (iBT) 9 (IELTS)
Sp 13	2	1	1	0	1	1	295 <sup>#</sup>	86
F 12	11	9	2	0	7	4	1150 (2) 308 <sup>#</sup> (9)	87
Sp 12	2	1	1	0	1	1	1135	
F 11	22	18	3	1	12	10	1108	
Sp 11	6	3	3	0	6	0	1146	
F 10	17	15	1	1	12	5	1121	94 iBT
Sp 10	4	2	2	0	4	0	1042	
F 09	16	15	1	0	8	5	1194	
Sp 09	2	2	0	0	2	0	1345/5.3	NA
F 08	14	12	2	0	10	3	1173/3.8	583

\*Anticipated, class not complete #New scale

**Table 21. Nationality Distribution of Incoming Students.**

Year	USA	China & Taiwan	India	Eastern Europe	Korea & Thailand	Others
F 14*	11	2	0	0	0	2
AY 13/14	11	2	0	1	0	5 (Africa, Bahamas, Sri Lanka)
AY 12/13	8	2	1	0	1	1
AY 11/12	13	6	2	0	0	3
AY 10/11	18	3	1	0	0	1
AY 09/10	14	3	2	0	0	1

\*Anticipated



**Table 22. Gender and Minority Status Distribution of Incoming Students.**

	<u>USA - Gender</u>			<u>Foreign - Gender</u>			<u>US - Minority</u>		
	Total	Male	Female	Total	Male	Female	African-American	Hispanic	Native-American/PI
F14*	11	5	6	4	2	2	0	0	1
AY 13/14	11	7	4	8	5	3	2	0	0
AY 12/13	8	4	4	5	4	1	1	1	0
AY 11/12	13	7	6	11	5	5	3	0	1
AY 10/11	17	10	7	6	4	2	3	0	0
AY 09/10	14	8	6	6	4	2	0	0	0

\*Anticipated, class not complete

**Table 23. Admission Success Rate<sup>#</sup>**

Year	Offers Made	Offers Accepted	Success Rate	Domestic Success Rate	Foreign Success Rate
F14*	42	15	36%	11/30 = 37%	4/12 = 33%
AY 13/14	31	18	58%	8/18 = 44%	10/13 = 77%
AY 12/13	28	15	54%	9/21 = 43%	6/7 = 86%
AY 11/12	38	23	61%	16/28 = 57%	7/10 = 70%
AY 10/11	33	23	70%	17/23 = 74%	6/10 = 60%
AY 09/10	36	16	44%	9/23 = 39%	7/11 = 64%

<sup>#</sup> Success rate may include loss of students because of denied visas.

\*Anticipated, class not complete

Our number of domestic applications declined slightly: 43 applications, seven (7) from Alabama. Our number of international applications, which was on the order of 150 per AY over the past decade, is now much lower (60 international applications for Fall 2014). We believe that this is part of a wider and ongoing trend: for example, as Chinese universities become better funded and equipped more Chinese applicants are electing to stay in their native country rather than accept offers to study in the United States. The entering class is being carefully selected by the Graduate Recruiting Committee (Street, Bonizzoni, Papish, Pan, Frantom, Goebbert, Rupar and Gupta) from these applicants.

The incoming fall 2014 class, as it stands, does appear to be reasonably diverse. Women, who had been traditionally underrepresented in our discipline, account for 8/15 of the class. We have been informed by the Dean's office (A&S) that for the purposes of the Dean's Diversity

Award women will no longer be considered “underrepresented”, reflecting the more recent demographic data for our discipline. One Pacific Islander student admitted for fall has accepted and will receive a Dean’s Diversity Award.

We have been involved in a variety of recruiting efforts. Profs. Street and Papish represented the Department at the regional SERMACS meeting. The department supported at least six recruiting trips for faculty visits to other departments regionally and nationally.

Multiple mailings were conducted to regional and national universities, to provide information on the Bama Grad Expo, to offer to present recruiting seminars to regional and national institutions, and to send literature to prospective students. We also hosted many of our domestic applicants for visits to our Department. Indeed, this past year significant travel funds were expended in recruiting. This included paying approximately \$1700 in application fees, mostly for domestic applicants. The payoff appears to be that we attracted a significant number of our first-round offers to the program, including two Graduate Council Fellowship and one Dean’s Diversity awardee. The average GRE score of the incoming class is at the newly established average.

### **Graduate Curricular Changes and Projects**

The Department is in the midst of a review and overhaul of our graduate curriculum. During the AY 2013-14, the Department instituted a new course, "Literature and Communication in Graduate Chemistry." This course grew out of a need recognized in our assessment studies to improve the written and oral communication skills of our graduate students. This course was offered in collaboration with Dr. Vincent Scalfani from UA Libraries in fall 2013. This course replaced the literature seminar requirement that is currently in place for second year graduate students.

The department held a “retreat” in December to discuss the structure of the graduate program. As a result of this conversation, work is underway to modify our candidacy exam requirement from the current “Original Research Proposal” to a dissertation research prospectus with a reduced original proposal requirement. In addition, we also reached consensus regarding a structured schedule of annual meetings of students with their dissertation committees. Finally, we agreed to begin development of a pair of core courses in graduate chemistry that would be taken by all incoming graduate students. One of these courses would focus on physical & analytical topics, and the other would cover organic/inorganic/biochemistry. The goal of these courses is to develop a basic graduate-level vocabulary in chemistry that would prepare students for the challenges of working in multidisciplinary environments.

## **VI. Summary of Faculty Service**

The faculty and staff continue to do a great deal of service for the College, University, state/national agencies, and professional organizations. Their service duties in the various categories are summarized below following a brief overview of departmental service duties.

### **Departmental Service:**

The Chemistry Department’s Committee Assignments for the 2013-14 academic year are shown below in Table 26 and 27. The four members of the Chair's Leadership Team are Snowden, Street, Woski, and Jennings, who have a heavier service load than typical faculty. Dr. Woski is the Director of Graduate Studies; he manages the graduate program and curriculum. Dr. Street is

**Table 26. Standing Department Committees 2012-13**

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<b>Executive Committee</b> K. Shaughnessy (Chair) S. Woski S. Street M. Jennings L. Busenlehner D. Dixon	<b>Long Range Planning and Alumni Relations</b> D. Dixon (Chair) M. Bakker R. Rogers A. Arduengo A. Gupta	<b>Undergraduate Curriculum</b> M. Jennings (Chair) L. Busenlehner J. Vincent G. Szulczewski D. Dixon S. Blackstock D. Leung
<b>Graduate</b> S. Woski (Chair) E. Papish R. Timkovich M. Bowman T. Snowden G. Szulczewski	<b>Graduate Recruiting</b> S. Street (Chair) P. Frantom D. Goebbert M. Bonizzoni E. Papish S. Pan A. Gupta P. Rugar	<b>Instrumentation</b> D. Nikles (Chair) C. Cassady M. Bowman R. Timkovich A. Arduengo R. Metzger R. Rogers
<b>Safety and Stockroom</b> D. Dixon (Chair) A. Gupta R. Rogers J. Vincent A. Arduengo	<b>Cava Lectureship</b> M. Jennings (Chair) R. Metzger S. Woski	<b>Arduengo Lectureship</b> T. Snowden (Chair) S. Blackstock
<b>Retention, Tenure, and Promotion Committee</b> C. Cassady (Chair) A. Arduengo M. Bakker S. Blackstock M. Bowman D. Dixon	A. Gupta M. Jennings R. Metzger D. Nikles E. Papish R. Rogers	T. Snowden S. Street G. Szulczewski R. Timkovich J. Vincent S. Woski
<b>SURP Committee</b> J. Vincent (Chair) S. Woski K. Shaughnessy C. Cassady G. Szulczewski		<b>Diversity Awareness Symposium Committee</b> Laura Busenlehner (Chair) Carolyn Cassady Patrick Frantom
<b>Other Service Roles</b> Website: K. Shaughnessy External Seminars: G. Szulczewski Graduate Student Seminars: R. Metzger Cumulative Exams: R. Metzger		EPR facility: M. Bowman NMR facility: R. Timkovich MS facility: C. Cassady X-ray facility: R. Rogers

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Director of Graduate Recruitment and Admissions and directs both the recruiting and admission of all graduate students into Chemistry. Dr. Jennings serves as Director of Undergraduate Studies and has a large task managing all of the undergraduate courses, teaching assistants, and the

undergraduate majors. Dr. Snowden serves as the Department's assessment coordinator. He has put in significant effort to establish measurable assessment criteria for the Department and our degree programs. Dr. Shaughnessy is the Department's webmaster. Dr. Szulczewski manages the external seminar program. Dr. Metzger manages the graduate student seminars and cumulative exams. Dr. Bowman (EPR), Dr. Timkovich (NMR), Dr. Cassady (MS), and Dr. Rogers (X-ray) supervise our major instrument facilities. Each plays a key role in ensuring this shared instrumentation remains in working conditions. Drs. Street (NOBCCChE), Woski (CGSO), Busenlehner (SCACS), and Shaughnessy (GSE) serve as advisors to departmental student groups.

**Table 27. Special Committees for 2013-14**

**Materials Chemistry Search Committee**

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S. Street (Chair)

A. Gupta

S. Pan

E. Papish

M. Weaver (Met. Eng.)

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**College Service:** Department faculty provide significant service to the College. Numerous department faculty serve on College committees including: College Technology Committee (Bonizzoni), Graduate Committee (Bowman), A&S Classroom Technology Task Force (Busenlehner), College Leadership Board Faculty Representative (Cassady), Technology and Research Working Group (Dixon), Committee for Academic Continuity (Frantom), Active Learning Initiative Mentor (Frantom), Chemical and Biological Engineering Head Search Committee (Gupta), A&S Scholarship Committee (Jennings), Diversity Committee (Leung, Pan), A&S Tenure and Promotion Committee (Snowden), Undergraduate Curriculum Committee (Szulczewski). Dr. Shane Street serves as the Ombudsman for the College. Chemistry again served as host to chemistry events in the Science Olympiad and provided demonstrations in the College tent at Homecoming on the Quad.

**University Service:** Department faculty serve on a wide range of University committees, including: UA Year of Energy Committee (Blackstock), Technology Research Advisory Committee (Busenlehner), Vice President for Research Search Committee (Cassady, Gupta), Association of Women in Science Advisor (Cassady), 3-Minute Thesis Judging (Cassady), Laboratory Safety Committee (Cassady), Burnum Award Committee (Dixon, Rogers), CBHP Admissions Committee (Dixon), SEC Faculty Award Committee (Dixon), Student Health Committee (Goebbert), Conflict of Interest Policy Committee (Gupta), CAF Users Advisory Committee (Nikles, Chair; Szulczewski), Intellectual Property Committee (Nikles), Council of Center Directors (Rogers), Radiation Control Advisory Committee (Rogers), Chemical Safety Committee (Rogers), Campus Laser Safety Committee (Street, Chair), Tri-Campus Materials Science Program Exam Committee (Street), RGC (Street, Area A Chair), Institutional Animal Care and Use Facility (Vincent, Vice-Chair), Laboratory Safety Committee (Vincent), Graduate Council (Woski).

Chemistry has a long history of active participation in the Faculty Senate. Drs. Vincent and Blackstock are currently serving on the Faculty Senate and Dr. Cassady serves as an alternate. Dr. Vincent is on the Faculty Senate Steering and Faculty Participation in the Selection of Deans

and Department Chairpersons, and Evaluation of Academic Programs (co-chair) committees. Dr. Blackstock serves as the senate representative to the University Textbook Committee.

Department faculty are also involved in the management of research centers on campus. Dr. Rogers is director of the Center for Green Manufacturing and Dr. Vincent is coordinator of the Center for Biomolecular Products. Dr. Nikles is the director of the Central Analytical Facility. Dr. Gupta is co-director of MINT and serves on several internal MINT committees. Dr. Blackstock served on the MINT facilities manager search committee. Dr. Rogers serves as the faculty advisor for the Mallett Assembly. Chemistry faculty served as judges for the UA Undergraduate Research and Creative Activity Conference (Bonizzoni, Pan, and Goebbert). Dr. Shaughnessy served as a faculty interviewer for the Undergraduate Fellows Experience program.

### External Service

**Local, State, and National Agencies:** Chemistry department faculty provide service to the following local, state, and national agencies: AMSTI Advisory Board (Bakker), Learning Labs Advisory Board, Alabama Museum of Natural History (Bakker), Alabama Science in Motion Steering Committee (Shaughnessy), Black Water River Keepers (Street), Jacksonville State University, Physical and Earth Sciences Review Committee (Street), Chemistry Committee, State of Alabama Articulation and General Studies Committee, STARS (Vincent), State of Alabama Radiation Advisory Board of Health (Vincent).

**Editorial and Advisory Boards:** Department faculty provide service to a number of organizations as members of advisory committees including: OWLv2 Advisory Board (Blackstock), the U. Chicago Center for EPR Imaging (Bowman), ALCF User Advisory Committee, Argonne National Lab (Dixon), User Executive Committee, Environmental Molecular Sciences Laboratory, DOE (Dixon), External Advisory Board of NSF Sponsored Center for Mathematical Achievement in Science & Technology at Grambling State University (Nikles), conference chair Gordon Research Conferences on Ionic Liquids and Crystal Engineering (Rogers), 6<sup>th</sup> International Congress on Ionic Liquids International Advisory Board (Rogers), 7<sup>th</sup> Green Solvents Conference Advisory Board (Rogers), Collaborative Conference on Crystal Growth Advisory Board (Rogers), DOE Joint Bioenergy Institute, UC Berkeley (Rogers). A number of department faculty serve on editorial or advisory boards to scientific journals including: *Journal of Analytical and Bioanalytical Techniques* (Bonizzoni), *Applied Magnetic Resonance* (Bowman), *Journal of Magnetic Resonance* (Bowman), *Spin Physics*, *Spin Chemistry*, and *Spin Technology* (Bowman), *Biochemistry* (Busenlehner), *International Journal of High Performance Computing* (Dixon), *Journal of Physical Chemistry* (Dixon), *Journal of Fluorine Chemistry* (Dixon), *Metallurgical and Materials Transaction* (Gupta), *Nanomagnetism* (Gupta), *Rare Metals* (Gupta), *Nature Scientific Reports* (Gupta), *Advances in Physical Chemistry* (Metzger), *The Chemical Record* (Metzger), *Chemical Letters* (Rogers), *Chemical Communications* (Rogers), *Green Chemistry* (Rogers), *Separation Science and Technology* (Rogers), *Solvent Extraction and Ion Exchange* (Rogers), *ChemSusChem* (Rogers), *Biological Trace Element Research* (Vincent), *Journal of Biomedicine and Biotechnology* (Vincent), *F1000 Research* (Woski). Dr. Rogers is Editor-in-Chief for the American Chemical Society journal *Crystal Growth and Design*.

**Professional Organizations:** Department faculty serve on committees for a range of professional science and education organizations: Chair, Asilomar Conference Committee, ASMS (Cassady), ACS Fellows Selection Committee (Dixon), Executive Committee, ACS Division of Fluorine Chemistry (Dixon), ACS Committee on Publications (Dixon), ACS Councilor for Division of Fluorine Chemistry (Dixon), National/International Symposia Chairs (Rogers (3), Vincent (1)), Spedding Award Committee, Rare Earth Society (Rogers), ACS Environmental Improvement Committee (Rogers), ACS E. V. Murphree Award in Industrial and Engineering Chemistry Selection Committee (Rogers), ACS Multidisciplinary Program Planning Group (Rogers), Basic Terminology of Crystal Engineering Committee, IUPAC (Rogers), AVS Magnetic Interfaces and Nanostructure Division Executive Committee (Szulczewski), Organizing Committee, 7<sup>th</sup> Conference on Metal Toxicity and Carcinogenesis (Vincent). Dr. Arduengo is the UA representative to the Alexander von Humboldt Foundation (Germany) and the Deutsche Akademischer Austausch Dienst (German Academic Exchange Service). Dr. Shaughnessy is the awards chair for the Alabama Section of the American Chemical Society. Department faculty also provided extensive service as reviewers for national and international journals and public and private funding agencies including NSF, NIH, DOE, ACS-PRF and many others. Faculty report reviewing in excess of 577 manuscripts, 7 books or book chapters, and 229 grant proposals or preproposals. Faculty served on 7 grant panels during the year.

**Consulting:** A number of Department faculty members serve as consultants: McGraw-Hill Higher Education (Bonizzoni), Cengage Publishing (Jennings), Argent Fox LLP (Rogers), Crowell & Moring (Rogers), Frommer, Lawrence, & Haup LLP (Rogers), Kenyon & Kenyon (Rogers), Reliance (Rogers), Winston Strawn (Rogers), Pearson Publishing (Street), Novus International (Vaid),

## VII. Summary of Outreach/Fundraising Activities

**Outreach:** The Chemistry Department and its faculty are actively involved in education and research outreach activities within the community. These activities include:

Chemistry Summer Research Experience for Undergraduates: Each summer, the Department of Chemistry hosts undergraduate students from around the country for the Summer Research Experience for Undergraduates. Dr. John Vincent and Dr. Stephen Woski organize this effort. In summer 2013, twelve students were chosen from over 100 applications to participate in the program. The program is funded by the National Science Foundation and provides outstanding undergraduate chemistry students with the opportunity to conduct high-level chemical research for 10 weeks with faculty researchers. Students receive payment as research assistants and housing, funded by the NSF grant. The program has been consecutively funded by the National Science Foundation since 1987 and has trained over 200 students. Follow-ups have shown that over 80 percent of the students who participated in the program go on to get their doctorate in chemistry. We are pleased to have recently learned that the NSF has renewed the department's REU funding.

Diversity Awareness Symposium: Dr. Laura Busenlehner organized the Diversity Awareness Symposium as part of her NSF CAREER award, which was held April 27, 2013. The Diversity Symposium highlighted the role of people from diverse backgrounds in science. Students and faculty from schools throughout the region were invited to participate. Approximately 70 people registered for the symposium. Prof. Abby Parrill (U. Memphis), Prof.

Pablo Sobrado (Virginia Tech), and Prof. Stefan France (Georgia Tech) served as the keynote speakers. Panel discussions were held on fostering diversity in the chemical sciences, support for underrepresented groups, and building collaborative research. A poster session with over 30 posters was held for student participants. NSF, A&S, and Chemistry provided funding for this symposium.

Materials Camp: Dr. Bakker helped organize a week-long Materials Camp that is run in partnership with the ASM International Education Foundation and the US Air Force. A total of 22 middle and high school science and mathematics teachers attended the camp in summer 2013. This camp focuses on hands-on demonstrations using common materials that teachers can do for and with their classes to illustrate fundamental science in the world around us.

Rural Entrepreneurial Internship Program (EIP): This program is organized by Dr. Karen Boykin and supported by an NSF NUE grant. The program sponsored 12 students from Hale and Green County. The students worked to develop start-up companies tied to green technologies incorporating concepts from nanobiotechnology in collaboration with faculty and mentors from UA and surrounding communities.

Rural Entrepreneurs of Alabama for Sustainability (REALaSus) Internship Program: The REALaSus program, which is run by Karen Boykin through the Center for Green Manufacturing, is a platform for training, developing, and growing student-based businesses in science and technology areas. The program is run in two rural Alabama towns, Moundville and Reform. Student participants develop ideas to use materials that can be locally sourced, such as bamboo, to develop new products that can be sold through student-run businesses. The program seeks to encourage students from these rural areas to consider pursuing careers in STEM-related fields.

High School Visits to UA: Dr. Bakker hosted the AP Chemistry classes from Central, Northridge, Hillcrest, Bryant, and Demopolis high schools on campus. The students spent a day in the freshman chemistry laboratories doing experiments and learning about opportunities to pursue chemistry and other STEM fields in college.

Visits to Schools: Several faculty visit local schools to perform chemistry experiments and talk about careers in science.

Science Olympiad: Each year, the Department hosts several chemistry events for junior and senior high school students in the regional Science Olympiad Event.

Homecoming on the Quad: Each year, Chemistry performs experiments with liquid nitrogen in the A&S tent during the Homecoming festivities. This event is always highly popular with children, and parents, as everyday items are flash frozen in liquid nitrogen.

**Fundraising Activities:** The department currently has four support funds for which it is actively seeking donors.

- Chemical Science Education and Research Endowed Support Fund
- Anthony J. Arduengo, III Endowed Lecture Series
- Michael P. Cava Endowed Support Fund
- M. V. Lakshmikantham Endowed Scholarship