

2014-2015  
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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Prepared by

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## One Page Summary

**Faculty Appointments:** Two new faculty, Dr. Jared Allred and Dr. Jack Dunkle, were hired as assistant professors beginning in fall 2015. Dr. Allred research specialty is solid state chemistry. Dr. Dunkle is a chemical biologist. Dr. Patrick Frantom was promoted to associate professor with tenure.

**Awards:** Faculty: Dr. David Dixon received the ACS Division of Fluorine Chemistry Distinguished Service award in recognition of his long service to this division. Dr. Timothy Snowden was named a top 10 reviewer for Elsevier organic and medicinal chemistry journals for 2014. Dr. John Vincent was named a fellow of the American College of Nutrition. Dr. Laura Busenlehner was named an A&S Distinguished Teaching Fellow and Dr. Patrick Frantom was named a A&S Distinguished Teaching with Technology Fellow. Graduate Students: Ashley Jolly was selected to the highly competitive ACS Division of Organic Chemistry Graduate Research Symposium. Joseph Meany placed 3<sup>rd</sup> in the UA 3-minute thesis competition. Undergraduate: Senior chemistry major Lynda Truong was a Goldwater Scholar this year.

**Teaching:** The Chemistry Department accounted for nearly 28,000 student credit hours, which was a 4% increase over AY 13-14. The median faculty member was responsible for 500 SCH during the academic year. The department had 259 undergraduate majors and 90 PhD students in 13-14. The department had 27 BS, 16 MS, and 14 PhD graduates in 2014.

**Research:** Department faculty have over \$10 million in current funding and received \$1.7 million in new funding during this academic year. Research expenditures totaled \$2.6 million in FY 14. The faculty submitted 75 proposals with a combined requested amount of \$21 million. The faculty published 115 peer-reviewed papers. In addition, the faculty published 13 patent applications, 7 issued patents, 2 books, and 3 book chapters. Chemistry faculty and students presented 160 talks at local, regional, national, and international scientific meetings and 48 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. Cassidy serves as an alternate senator. Dr. Vincent serves as chair of the Laboratory 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. 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 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. Kevin Shaughnessy was co-organizer of the first UA-NOYCE summer internship for students interested in teaching high school science and math. Fifteen students from UA and regional community colleges participated. Ten undergraduate students from around the country participated in the 2014 Research Experience for Undergraduates program. The Chemistry department hosted the 2015 Southeastern Chemistry Undergraduate Research Conference in February. Fifty undergraduate students from seventeen regional schools gave presentations during the meeting.

## 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. Patrick Frantom was promoted to associate professor with tenure this year. The Department is pleased to have recruited two outstanding new faculty members who will join the faculty in fall 2015. Dr. Jared Allred earned a BS degree at Case Western Reserve University and a PhD at Princeton University. He is currently a post-doctoral appointee at Argonne National Laboratory. His research focuses on novel solid state inorganic materials. Dr. Jack Dunkle earned his BS degree at UAB and a PhD at UC-Berkeley. He is currently a post-doctoral associate at Emory University. Dr. Dunkle's area of research is chemical biology with a focus on understanding the structure, mechanism, and function of RNA polymerase enzymes.

**Faculty Departures:** The department lost two colleagues during this academic year. Dr. Robin Rogers resigned from UA to accept the Canadian Excellence Research Chair in Green Chemistry at McGill University. Dr. Laura Busenlehner passed away in the fall semester.

**Faculty Awards:** Dr. David Dixon received the ACS Division of Fluorine Chemistry Distinguished Service award in recognition of his long service to this division. Dr. Dixon also received the Outstanding International Paper Award from Pleiades Publishing for the most original paper published their journals in 2013. Dr. Robin Rogers was named a Highly Cited Research by Thomson-Reuters, which signified he was in the top 1% of chemistry researchers based on citations. Dr. Timothy Snowden was named a top 10 reviewer for Elsevier organic and medicinal chemistry journals for 2014. Dr. John Vincent was named a fellow of the American College of Nutrition. Dr. Laura Busenlehner was named an A&S Distinguished Teaching Fellow and Dr. Patrick Frantom was named a A&S Distinguished Teaching with Technology Fellow. Dr. David Dixon received the This is How College is Meant to Be award from Dean Olin for his mentorship of students.

### Individual Faculty Highlights

**Dr. Anthony Arduengo** – Professor Arduengo continues to represent UA interests with international institutes and 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 chaperoned a student study-abroad Semester for 2 UA undergraduates in Chemistry at the Johannes Gutenberg University of Mainz, Germany. In exchange, the Arduengo laboratory in Tuscaloosa was host to five German student scholars from Mainz, Marburg, Clausthal, and Erlangen, Germany. 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. The third and fourth German students from Mainz just recently arrived in Tuscaloosa for their exchange studies. During the course of the most recent study-abroad Semester, Professor Arduengo was approached by Georgia Tech, and Virginia Commonwealth University about the possibility of including Tech and VCU students together with UA students

for an overseas experience in 2016. Plans to facilitate this broader, multi-University study abroad experience are currently underway. Professor Arduengo continues to operate 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.

Professor Arduengo represents UA prominently on the international stage. Work from his research group continues to appear in highly visible journals world-wide. In January 2015, he was the special awardee of a guest professorship at the Johannes Gutenberg University Mainz and the Max Planck Institute for Polymer Research (CINEMA, the Center for INnovative and Emerging MAterials). Professor Arduengo was also one of select group of international dignitaries invited to present at the International Research and Training Group - Münster-Nagoya in the Winter of 2014. He has been re-invited to present a plenary lecture at the ImSat-12 meeting in Goslar, Germany in the fall of 2015. Professor Arduengo has accepted a number of invitations to author special articles in prestigious and internationally recognized scientific journals during the coming academic year.

Together with Professor Opatz in Mainz, Professor Arduengo has formed a research and development consortium to establish a new industrial chemical infra-structure. The StanCE (Technology for a Sustainable Chemical Economy) consortium seeks to develop a chemical economy that is based on a renewable and flexible resource, wood. Not only will StanCE technologies enable a revolution in chemical manufacturing, but it places one of Alabama's important and abundant resources, wood, at the forefront of this revolution. StanCE is off to a strong start with partners in the U.S., Germany, Canada, England, and Japan. Local UA-side startup funding has been achieved through a GRC grant and federal applications are in progress. Discussions with several business partners have been initiated already and are in various stages of formulation. Federal funding for StanCE's Japanese partners is now in place.

**Dr. Martin Bakker** - This year saw the publication of five papers and the submission of a sixth. Two papers were collaborative with groups outside UA: one in polymer composites with an engineering group and a small business at Michigan State University, the other with a long time collaborator in Finland. The other four papers were in hierarchically porous monolithic catalysts, and represent a significant extension of our porous materials work by demonstrating applications of these materials. This year also saw the graduation of Dr. Katrina Staggemeier, and the fifth summer of a successful and well received Materials Camp for 22 area science and mathematics teachers, as well as six prospective student teachers in the Noyce program.

**Dr. Silas Blackstock** supervised 4 graduate students (Melody Kelley, Carl Saint-Louis, Chinenyeze (Izzy) Nwankwoala, and David Warner) and 3 undergraduate students (Lauren Hagler, Savannah Reach, and Kip Callahan). Melody completed her PhD degree in December 2014. Lauren (an ACS Scholar) and Savannah completed ACS BS Chemistry degrees in May 2015. Lauren will enter the PhD chemistry program at Illinois in the fall and Savannah will complete her UA MS chemistry degree this summer and attend a graduate dance program at UC-Irvine in the fall. Carl was awarded an SREB fellowship for AY 2014-15. Dr. Blackstock taught CH232 (organic 2) in the Su14, F14, and S15, and taught CH435/531 (physical organic chemistry) in the S15. In research, the group continues to develop redox auxiliary catalysis as a new way to activate and trigger organic reactions and a patent on this methodology was filed and is pending. The group gave 4 research presentations in the past year. Dr. Blackstock has been invited to speak this June at the Physical Organic Chemistry Gordon Research Conference. Dr.

Blackstock served on the faculty senate, the UA QEP committee, and as faculty advisor for the UA ACS student affiliates group.

**Dr. Bonizzoni** - In the last academic year Dr. Bonizzoni published multiple papers, two of which appeared in particularly high-impact journals, i.e. the Journal of the American Chemical Society, the premier publication worldwide dedicated to the chemical sciences, and Macromolecules, the highest-impacting publication in the field of macromolecular science. Dr. Bonizzoni also submitted multiple external grant applications, including submissions to the NSF's CAREER program, and a multi-campus submission to the EPSCoR program in collaboration with the University of Southern Mississippi, Mississippi State, and UAB. Dr. Bonizzoni was selected to be the UA campus applicant for the Dreyfus Teacher-Scholar award. Dr. Bonizzoni's group grew to include four graduate students and four undergraduates. The group expanded their focus from the binding of small molecules onto hyperbranched polyelectrolytes to applications of these macromolecules to chemical analysis.

Dr. Bonizzoni taught the undergraduate first- and second-semester Organic Chemistry series in the fall 2014 and spring 2015 semesters respectively (ca. 310 students overall). Previously adopted learner-centered instruction techniques were refined, and a heavier use of technology was introduced in the classroom, especially with heavier use of the College-provided iPad as a teaching and content-creation tool.

Dr. Bonizzoni continued his service 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, for funding applications for the NSF. Dr. Bonizzoni also organized and conducted a professional development workshop for high school teachers in the chemical sciences centered on food chemistry as a medium to enhance chemical education at the high school level.

**Dr. Bowman** – not provided

**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 have been in the group in the past year, plus one undergraduate researcher. Dr. Logan Feng obtained his PhD in December 2014 with research in the area of electron transfer dissociation of peptides. In the past year, several presentations of the group's work were given at the 62<sup>nd</sup> Annual American Society for Mass Spectrometry conference in Baltimore and the Southeast Regional American Chemical Society Meeting in Nashville. Dr. Cassady was also a keynote speaker at the International Workshop on MS-Based Proteomics, Bioinformatics and Health Informatics in Turkey, which celebrated the German-Turkish Year of Science. During the past year, the group has been very fortunate to have continuing funding from both NSF and NIH. The NSF grant deals 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 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 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 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, which involves the development of iron oxide nanoparticles as matrices for matrix-assisted laser desorption ionization (MALDI) mass spectrometry, has recently been the subject of a US patent. In addition, Dr. Cassady lead a group of 14 UA faculty in submitting a proposal to NSF’s Major Research Instrumentation (MRI) program for acquisition of a multi-user Fourier transform ion cyclotron resonance mass spectrometer; the result of this submission should be known in summer 2015. Dr. Cassady’s teaching assignment in fall 2014 was CH 223, Quantitative Analysis. In spring 2015, she taught the graduate course CH 526, Chemometrics, to a class of 6 graduate students. She was also very involved in service activities. She continued her work as faculty supervisor for the mass spectrometry facility. In addition, she is working closely with students to get the new UA-Tuscaloosa Association for Women in Science affiliate group up and running. Dr. Cassady is also chair of the departmental Retention Tenure and Promotion (RTP) Committee.

**Dr. David Dixon** – During the 2014-2015 academic year, Dr. Dixon was involved in a variety of research, teaching, and service activities. He taught CH-341 Physical Chemistry in the fall 2014 semester. He also taught CH-549, Advanced Physical Chemistry II, Atoms and Molecules at the same time. Using the remaining HHMI funding, he developed Millikan oil drop experiment and a Franck-Hertz experiments for CH-117 (Honors Introductory Chemistry) and these were implemented for the first time. He ran the computational chemistry lab for CH-117 in fall 2014. He taught a Freshman Learning Community on Energy and the Environment in fall 2014. 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 6 undergrad research students during the fall 2014 semester and 2 CBHP students, 8 undergrad research students, and 1 Emerging Scholar in the spring 2015 semester. He mentored 1 high school intern in his laboratory in Summer 2014. His students received 3 UA Randall Research Awards in April 2015. Dixon served on the Departmental Undergraduate Committee, advised undergraduate students, served on the 2015 CBHP selection committee, served on the Departmental Long Range Planning Committee, served on the Departmental Safety Committee, and served on UA’s Burnum Award Committee. He was the Chair of the TRAC technology committee for the VP of IT. He serves as the sole ACS Councilor for the Division of Fluorine Chemistry and is a member of the Division Executive Committee. He is an Associate of the ACS National Committee on Publications. He is on the Advisory Board of the *Journal of Physical Chemistry* and the Editorial Boards of *The International Journal of High Performance Computing*, *Computational and Theoretical Chemistry*, and the *Journal of Fluorine Chemistry*. He completed his term on the User Executive Committee of the William R. Wiley Environmental Molecular Sciences Laboratory at PNNL. He is on the User Advisory Board of the Argonne Leadership Computing Facility and of the Oak Ridge Leadership Computing Facility. He serves as a reviewer for many journals as well as funding agencies. He ran the 22<sup>nd</sup> Winter Fluorine Conference in January 2015 and organized the ACS Fluorine and Iodine Award Symposia at the National ACS meeting in Denver in March 2015. He received the 2015, Distinguished Service Award, Division of Fluorine Chemistry, American Chemical Society.



In 2014-2015, the research group had 5 graduate students and 5 post-doctoral fellows. Ted Garner (August 2014) and Tanya Mikulas (May, 2015) received PhD degrees. There are two DOE Office of Science grants in catalysis (through PNNL and UC-Davis (complete)), 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. Cassidy 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 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 efforts there. A computational sciences Grand Challenge proposal to the MSC/EMSL at PNNL in catalysis received ~1,500,000 node hours of computer time on the latest EMSL computer for two years. This supports a team of scientists from multiple universities and national labs. Smaller EMSL Science Theme proposals continue to receive modest blocks of computer time. An INCITE proposal for 150,000,000 hours in the area of heavy element chemistry received an allocation for a second year. This supports a team of scientists funded by DOE from multiple universities and national labs. An EFRC proposal with Georgia Tech as the lead in the area of reactions and sequestration of acid gases was funded.

He is a co-PI on a proposal to DOE's NEUP on designing molecules for separation of actinides and lanthanides led by Tennessee Tech. He is a co-PI on renewal proposals for his catalysis and geochemistry projects through PNNL. He led an unsuccessful proposal for UA for Beckmann Scholars.

Dr. Dixon had 19 papers published or accepted. A number of papers have been submitted and were accepted post the 03/31/2015 deadline. He had 10 invited presentations. His Hirsch index is ~75.

Research efforts include work in computational catalysis, geochemistry, nanoscience, actinide chemistry, chemical hydrogen storage, and main group chemistry. Research highlights include:

- Continued work on CCSD(T) and DFT calculations of catalytic reactions on transition metal oxides. Determined the potential energy surfaces for the dehydrogenation, dehydration, and ether formation catalytic reactions of multiple alcohols on transition metal oxide complexes. Developed a new mechanism based on combining Lewis/Brønsted acid-base properties. Showed that high level correlated methods are needed to explain experimental results. Extended work to polyols and acids. Initiated new work on RuO<sub>x</sub> and OsO<sub>x</sub> clusters;
- Continue to calculate extensive set of thermodynamic properties of biomass intermediates;
- Continuing to predict the properties (structures, spectra, energetics) of boron-nitrogen heterocycles for chemical hydrogen storage applications with Boston College and PNNL;
- Developing models for the activation of CO<sub>2</sub> and H<sub>2</sub> by frustrated Lewis acid-base pairs;
- Continued work on single site metal ion catalysts encapsulated in the acid site of a zeolite. Extended studies to more ligand exchange reactions and to metal clusters in the site. Extended work to include Ir and Os with UC Davis and UC-Berkeley;

- Continue predictions of the properties of iridium carbonyl clusters. Studying phosphine and carbene substitution in iridium carbonyls;
- Continued extensive collaboration with Russian group on radiation (alpha, beta, gamma, intense IR, proton) damage in fluoropolymers;
- Developed mechanism for cluster formation in solution for M(IV)hydrated ions. Focus is on how hydrogen ions are lost and the role of oxolation vs ololation reactions;
- Calculating acidities of substituted amino acids and polypeptides. Calculated acidities and other properties of phosphorylated amino acids;
- Continuing studies of reactions of lanthanide atoms with a focus on H<sub>2</sub>O/H<sub>2</sub>O<sub>2</sub> reactions to explain results from the L. Andrews group at the University of Virginia;
- Use novel cluster growth algorithm to find the global minimum for (MgCO<sub>3</sub>)<sub>n</sub>. Expand to Ca clusters. Developed new method to predict heats of formation of minerals based on accurate cluster energies in the gas phase and extrapolation to the infinite cluster limit;
- Developing database of transition metal compound heats of formation to improve parameterization of SEMO methods for large molecules. Developing new diagonalization methods for massively parallel computers for large molecular systems;
- Extensive studies of CN/NC substitution at U as well as reactions of U and Th with other small molecules; and
- Continuing studies of CO<sub>2</sub> reactions with cations and model minerals in aqueous solution. Predict spectroscopic properties and energetics.

**Dr. Frantom** - Over the 2014-2015 academic year, research in Dr. Frantom's laboratory was supported through an NSF-CAREER award (2013-2018) and an NIH R01 award (2015-2019). This funding supported research efforts of seven graduate and four undergraduate researchers. During this year, four RA positions were supported (2 NSF CAREER Award, 1 UA Graduate Council Fellowship, and 1 NSF Graduate Research Fellowship). Undergraduate research support came from the Computer-Based Honors program and dedicated funding from the NSF CAREER award (1 summer student and 3 academic year positions). The laboratory published four peer-reviewed publications (2 in *Biochemistry*, 1 in *Archives of Biochemistry and Biophysics*, 1 in *BBA-Proteins and Proteomics*). A highlight of the year was Dr. Frantom's visit to the University of Havana in Cuba to teach undergraduate biochemistry students and interact with researchers at the Center for Protein Studies. Research from the Frantom laboratory generated seven poster presentations at regional and national conferences. Dr. Frantom gave invited lectures at Florida State University, Marquette University, UA-Huntsville, and Wesleyan University. Dr. Frantom served as a mentor for the Active Learning Initiative sponsored by the College of Arts and Sciences. Dr. Frantom also served as an NSF panelist and ad hoc reviewer for multiple scientific journals.

**Dr. Daniel Goebbert** - The Goebbert group currently consists of 4 graduate students and 7 undergraduate students. In the last academic year the group published several manuscripts. The group has sought outside funding from the National Science Foundation, Army Research Office, Department of energy and the American Chemical Society Petroleum Research Fund (results still pending). Dr. Goebbert was supported for part of the year by a CARSCA grant. Dr. Goebbert taught CH117 in the fall and implemented several new learner-centered techniques and assessment tools. Dr. Goebbert taught physical chemistry lab in the spring. Dr. Goebbert served

on the Graduate recruiting committee for the department, participated in the Science Olympiad and assisted with the Southern Undergraduate Research Conference. He also served on the university student health committee. Dr. Goebbert reviewed multiple manuscripts, proposals and reviewed a new textbook.

**Dr. Arun Gupta**

- Taught Undergraduate Physical Chemistry II Course (CH 342) in spring 2014.
- Advisor for six PhD students and one post-doctoral associate.
- Served on several department and university-level committees. Associate Director of the MINT Center. Editorial Board of Nature Scientific Reports and Rare Metals Journal.
- Actively involved in research with 14 refereed articles appearing in print; 8 additional articles accepted or awaiting publication decision.
- Total of over 375 refereed journal publications with more than 15,000 citations. H-index of 64.
- Continued research funding through several awards: DOE, NSF-ECCS, NSF-CHE, and NSF-IS&E.

**Dr. Jennings** - With regards to academic service, Dr. Jennings instructed CH 432 and 532 in the fall of 2014. In the spring of 2014, Dr. Jennings instructed CH 237. Based on evaluations (student) for both CH 532 and 237, he received high marks from the undergraduate and graduate 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 (3 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, (-)-aspergillilide 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 carbocyclization of  $\alpha,\beta$ -acetylenic esters with a variety of Grignard reagents for vicinal functionalization protocols. During the past academic 2014-2015 year, Dr. Jennings has given 1 professional presentation and published 2 manuscripts. 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 numerous proposals for NSF and ACS-PRF.

**Dr. Diana Leung** - During the Summer 2014, Dr. Leung taught Organic Chemistry I (CH 231, 91 students) and Organic Chemistry Laboratory I (CH 237, 32 students). During the fall 2014, Dr. Leung taught two sections of General Chemistry I (CH 101, 422 students), Organic

Chemistry Laboratory I (CH 237, 161 students), and Organic Chemistry Laboratory II (CH 338, 43 students). During the spring 2015, Dr. Leung taught Organic Chemistry I (CH 231, 194 students), and two sections of Introductory Organic Chemistry (CH 105, 305 students). Overall, Dr. Leung was responsible for 4255 student credit hours in the last academic year.

Instructional technologies were integrated throughout these courses to enhance the students' learning experience; technologies used included *Blackboard Learn* and online homework through the Cengage's *OWL*, Pearson's *Mastering Chemistry*, McGraw-Hill's *Connect*. Dr. Leung also participated in academic continuity exercises during the spring 2015, when multiple class meetings were cancelled due to inclement weather. Dr. Leung used the app *DoodleCast Pro* on the iPad to deliver recorded lectures providing an experience similar to that of following a whiteboard lecture in the classroom. The lectures were distributed to students through the existing *Tegrity* streaming framework, allowing students to view the video at their convenience.

Dr. Leung served on the departmental Undergraduate Curriculum Committee, and the College's Diversity Committee, through which she was involved in the organization of the Capstone Recruitment Day for diversity oriented recruiting in high schools serving students with disadvantaged backgrounds in Tuscaloosa County and the surrounding Black Belt.

**Dr. Robert Metzger** - The Metzger group published a major research review paper in *Chemical Reviews*, failed to get an NSF grant, but has gathered experimental data for three new rectifiers, and has submitted a Communication the first rectifier for publication in the *Journal of the American Chemical Society*. Three posters were prepared for an International Conference in Jerusalem, Israel.

The critiques of the reviewers who did not fund our proposals will be met by new work done somehow somewhere, in collaboration if necessary. This group has two talented students and a steely determination to continue making its mark on the world regardless of the deplorable funding climate in the United States.

**Dr. David Nikles** - I taught CH 101 (fall semester) and CH 102 (spring semester), with each class having about 200 students. I also team taught a new course, NEW-490, Introduction of Nanotechnology and its Societal Impacts. This year I published one manuscript in the *Journal of Magnetism and Magnetic Materials*. Brian Goodell, one of my undergraduate research assistants was awarded a Goldwater Scholarship. Lindsey Cobb and Morgan Whitaker were awarded Randall Outstanding Research Awards. Morgan also won the top award for her poster presented at the 2014 University of Alabama System-Wide Honors Day. I submitted two grant proposals to the Department of Defense Congressionally Mandated Medical Research program to support basic research on drug delivery systems targeted to cancer stem cells. I was co-PI on a proposal to the NSF Major Research Instrumentation Program to acquire upgrades to the transmission electron microscope including a Si Drift Detector for Energy Dispersive Spectroscopy; rapid (<1 sec.) in situ TEM holder for annealing studies; in situ indentation TEM holder for nano-mechanical studies. I was a member of the program committee for the 2014 NanoBio Summit held at the University of Alabama. I presented an invited paper "Building and Managing a Multidisciplinary Materials Research Science and Engineering Center at the University of Alabama" at the summit. I ran a CAF workshop on "Building and Managing a Multidisciplinary Materials Research Science and Engineering Center at the University of Alabama". The purpose was to make the materials research faculty aware of the next MRSEC competition in 2016 and work toward submitting a competitive preproposal in the early fall of 2016.

**Dr. Shanlin Pan** - Dr. Shanlin Pan taught quantitative analysis and graduate course electrochemistry this year. He developed five new electrochemistry labs for the graduate electrochemistry class in order to enhance students' learning of electrochemistry methods and principles. Dr. Pan has applied Tegrity, clicker and blackboard systems for improving his students' learning outcomes in his quantitative analysis class. Dr. Pan supervised 8 graduate students and 9 undergraduate researchers and served on the dissertation committees of 19 students from chemistry and engineering. Dr. Daniel Clayton (PhD 2014) of the Pan group has successfully secured a tenure-track assistant professor position in Minot State University. Dr. Caleb Hill (PhD 2014) of the group has been productive in his quantum electrochemistry study with Professor Allen J. Bard in UT-Austin. Along with the Street group the Pan group has published Caleb's last work on single nanoparticle spectroelectrochemistry in *Journal of Physical Chemistry*. The 5<sup>th</sup> year student Jue Wang has successfully defended his dissertation and plans to graduate in this summer while searching for a job. The fourth year graduate students Jia Liu and Zhichao Shan have been very productive as they move toward their graduation. Both of them passed their proposal defenses this year. Jia Liu has published his single molecule work in PCCP and will present another excellent paper on ECL in NanoFlorida conference organized by PCCP in this summer. This paper has been submitted to a new journal ACS photonics. Zhichao Shan has proved that our NanoCOT catalytic electrode for solar water oxidation can be further improved by sensitizing its surface with more catalytic nanostructures. The 2<sup>nd</sup> year student Nelly Kaneza has been working on BODIPY dye sensitized solar cell along with a long-term collaborator Professor Haiying Liu from Michigan State and the 1<sup>st</sup> year graduate student Wilson Ma, whose father is an excellent polymer chemist in China, joined the group in spring and has started his single particle electrochemistry experiment. The group has been very aggressive in advising 9 undergraduate researchers in the past year. Six outstanding undergraduate researchers presented their work at the recent UA undergraduate research conference. Two of the undergraduate researchers Scott Rogers and Christian Palmer have published their work in the UA's undergraduate research journal Joshua.

**Dr. Elizabeth Papish** - *Research*: In the past academic year, Dr. Papish submitted 6 (4 external, 2 internal) proposals totaled at over \$1.3 million. She has had an active NSF CAREER award in force during the past year, and this April she received funding as lead PI from UA RGC for a level 2 collaborative grant on an anticancer project with co-PI John Kim of ChBE (\$150k total to be shared with both PIs). Research productivity has included two published papers, two submitted papers, and one manuscript in preparation. The most significant published work was a full paper on copper complexes for water oxidation in *Inorganic Chemistry*; water oxidation with copper is a new field and this work involved collaboration with the Pan and Bowman groups. Papish gave 7 invited research seminars at universities and colleges, and Papish or her students gave 7 conferences presentations. Papish advised 5 graduate students, 11 undergraduate students (including two REU students), and two postdoctoral fellows during the past academic year. Many of these students have won awards or fellowships. *Teaching*: In the area of teaching, Dr. Papish taught CHEM 413 and 501 and received favorable reviews. Significant efforts were put into revising the lab experiments and providing the students with schlenk lines to practice air sensitive synthesis techniques in the laboratory. The students made the "Grubbs" metathesis catalyst and were able to test it in catalytic ring closing metathesis (RCM), cross metathesis (CM), and ring opening metathesis polymerization (ROMP) reactions, which in some cases used

green solvents. These reactions were developed using recent chemical literature. The students, based upon survey data, enjoyed the lab experience. *Service*: Papish served on the GRC and has led efforts to enhance our graduate recruiting efforts via faculty visits (by both encouraging us to visit more schools and by doing several recruiting visits herself). Papish also led efforts to organize the Southeastern Undergraduate Research Conference (SURC) which serves an opportunity for regional undergraduates to share science results and it offers a recruiting opportunity for UA. Papish also engaged in several other mentoring and outreach activities with an emphasis on serving as a mentor both at UA and to women in science nationally. Papish served as a reviewer for several journals and for funding agencies, including an NSF panel in the past year. Papish began managing the XRD facility in January 2015 with the assistance of her postdoctoral fellow, Dr. Deidra L. Gerlach. *Entrepreneurship*: Papish has one patent application pending and another filed recently. Papish participated in the Crimson Startup Canvas in 2015 through AIME, but has decided to defer starting a company while more data is gathered. Nonetheless, the experience was very informative.

**Dr. Paul Rupar** - Dr. Rupar's SOI from Chemistry 101-001 (spring 2014) continued to improve (Course 3.810, Instructor 4.279). In fall 2014, Rupar developed and taught a graduate course (605-001) on polymer chemistry; students' reception to the course was extremely positive. For his spring 2015 101 class, Dr. Rupar used a number of innovative teaching methods, including a flipped classroom, delivering review sessions via Blackboard Collaborate, providing students with problem solving videos, and the incorporation of ChemWiki, an open source chemistry textbook.

The Rupar Group's first paper was accepted for publication in the journal *Macromolecular Rapid Communications*, a leading polymer journal. We are currently writing the draft for our 2<sup>nd</sup> manuscript and data for papers two additional papers are being collected. Rupar presented invited talks at the ACS meeting in San Francisco and the SERMACS meeting in Nashville.

Dr. Rupar submitted 2 proposals to the NSF. The first proposal was a solo-PI submission to CHE-MSN titled "The Design and Synthesis of Electron-Deficient Boron Containing Conjugated Polymers" for \$400K. The second proposal was as a co-PI submitted to DMR-SSMC titled "Investigating structure-property relationships in nanowire-polymer hybrid thermoelectric materials" for \$420K. Dr. Rupar submitted a proposal to the Beckman foundation for \$700K titled "The Synthesis of Polyethyleneimine Block Copolymers". Dr. Rupar's DNI-PRF proposal titled "The Living Anionic Polymerization of Functionalized Aziridines" was funded for \$110K over 2 years (the start date is 09/01/15).

Rupar served as a judge for the Undergraduate Research and Create Activity Conference, was a NSF-DMR Ad-hoc reviewer, and was a presenter at the Rodgers Library "Lightning Talk" lecture series. Dr. Rupar also worked with Science in the Classroom, a joint AAAS and NSF project, to transform articles published in the journal Science into educational resources.

**Dr. Kevin Shaughnessy** - The Shaughnessy group research focuses on the application of transition metal catalysts in organic synthetic reactions. The Shaughnessy group had five papers published this year. A paper published in the *Journal of Organic Chemistry* was highlighted in the journal *Organic Process Research & Development*. A volume of the book series *Organic Reactions* written by Dr. Shaughnessy over the past several years was published this year along with another book chapter. The Shaughnessy group gave a total of 6 presentations at regional, national, and international meetings and Dr. Shaughnessy presented two invited seminars. Dr.

Shaughnessy is PI of collaborative two NSF grants (with Dr. David Dixon and with Dr. Ryan Hartman, ChE) from NSF (\$700K total) and is PI for a subcontract from Thrupore Technology (\$40K). He was co-PI (with Dr. Tim Snowden) on an NSF-RUI grant that is subcontracted from Southeastern Louisiana University (\$39,000). He is also co-PI on an NSF-Noyce grant with 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 taught two lecture courses this academic year—Organic Chemistry I and II (CH 231 and 232) as well as numerous research and independent study courses in line with the standard load for chemistry. Dr. Shaughnessy generated over 1,100 student credit hours this year. Dr. Shaughnessy continued to receive very high student evaluations of his teaching. Dr. Shaughnessy currently mentors a group of five graduate students and a post-doctoral researcher. Dr. Shaughnessy mentored eight undergraduate research students this year. 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 Department of Mathematics Chair search committee, REU program 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 41 grants and manuscript.

**Dr. Timothy Snowden** - Dr. Snowden mentored five graduate students (Zhexi Li, Jordan Entrekin, Yinghui Liu, Brent Wells, and new student Jack Albert) and six undergraduate researchers during the 2014-15 academic year. Dr. Snowden taught CH 231 Organic Chemistry I during the fall semester and CH 405/505 Medicinal Chemistry in the spring, thereby accounting for 761 student credit hours. He received high Student Opinions of Instruction scores in both courses and was nominated for a UA National Alumni Association Outstanding Commitment to Teaching Award and for a UA College of Arts and Sciences Distinguished Teaching Fellowship. The Snowden group published one manuscript related to new strategies and methods for organic synthesis supported by an NSF CAREER Award. A second project funded through the same grant was completed in 2015, and the corresponding manuscript is in preparation. In addition, the Snowden group assisted in the completion of a collaborative project with Southeastern Louisiana University Professor Debra Dolliver and UA Professor Kevin Shaughnessy, thereby resulting in a joint publication. As Department Assessment Coordinator, Dr. Snowden devised the 2014-2015 Chemistry Department Assessment Plan and prepared the 2013-2014 Chemistry Annual Assessment Report with outcomes for over 100 assessment measures. Dr. Snowden chaired and co-organized the Anthony J. Arduengo, III Lecture in Main Group Element & Physical Organic Chemistry held in April 2014. He also served as a member of the UA College of Arts & Sciences Tenure and Promotion Committee for a third year and as a continuing member of the Department of Chemistry Graduate Committee. In addition, he reviewed manuscripts for all major scientific publishers, and, notably, was selected as an international *10 Best Reviewer in 2014* by Editors of the five Elsevier organic and medicinal chemistry journals. Dr. Snowden reviewed grant proposals for the ACS Petroleum Research Fund as well as forthcoming medicinal chemistry textbooks for two top publishers.

**Dr. Shane Street** - The Street group published two papers and another two papers are in near-final form to be submitted. I am co-PI on an educational grant currently in effect, an Alabama AMSTI training program, and senior personnel for the department's NSF-REU program. I was also senior personnel for a recently completed DoD SBIR project. I submitted a single investigator proposal on chemical ordering in metallic nanoparticles to the NSF which was not recommended for funding this round.

I taught three lecture courses in the reporting period, the standard teaching load for the fall and spring and another in Summer I. In fall, I taught a Honors General Chemistry (CH 117), to 139 students. In spring 2015 I taught Surface Analytical Techniques (CH 626) with an enrollment of five graduate students. I am chair of the dissertation committee for three graduate students (two of them co-advised) and supervise the research of three 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 12 other students.

I served on six University committees and three Departmental committees. I just completed my term as an A&S ombudsman, I am 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 successful faculty search committee for the Department in the area of materials chemistry. Other service includes manuscript reviews for seven peer-reviewed journals and grant reviewing for the NSF. I serve on the advisory board of Blackwarrior Riverkeeper.

I am the Director of Graduate Recruiting for the Department.

**Dr. Gregory Szulczewski** - The Szulczewski group continues to work in the areas of organic spintronics and thermoelectrics. Six peer reviewed manuscripts were published. Our manuscript entitled "Temperature dependent thermopower and electrical conductivity of Te nanowire/PEDOT:PSS microribbons" was chosen as an "Editors Pick" and another manuscript entitled "Temperature Gradient Approach to Grow Large, Preferentially-Oriented TIPS Pentacene Crystals for Organic Thin Film Transistors" was chosen by the editor for the journal cover art. Dr. Szulczewski gave invited seminars Mississippi State and the University of Mississippi. In the fall semester of 2014 Dr. Szulczewski taught CH 101 and CH102 (General Chemistry) in the spring semester of 2015 he taught CH 424 (Instrumental Analysis). Dr. Szulczewski mentored 3 graduate students (Ed Ellingsworth, Kim Anderson, and Tabatha Sutch) and 1 undergraduate student in research. In addition, he served on 19 Ph.D. committees and advised 42 undergraduates. Dr. Szulczewski served on four departmental, three university committees, and one MINT committee. Dr. Szulczewski reviewed numerous manuscripts for journals including Advanced Materials Interfaces, Journal of Physical Chemistry, Applied Surface Science, Journal of Applied Physics and Sensors. Dr. Szulczewski was a judge at the Southeastern Undergraduate Research Conference. Dr. Szulczewski served as the 2014 co-chair of the Magnetic Interfaces and Nanostructures Division of the American Vacuum Society and is currently serving as the 2015 program chair.

**Dr. Russell Timkovich** - The thrust of current research in the Timkovich group is determining the three-dimensional structure of biologically important proteins by nuclear magnetic resonance. The main goal now is the catalytic domain of the exoenzyme Zoocin A, which has potent antimicrobial activity against a broad spectrum of organisms. Our collaborator Dr. Gary Sloan and his group genetically engineered a mutant of this protein replacing cysteine 74 with an alanine. This mutant termed C74A still has full biological activity but is incapable of



forming intermolecular dimers via a disulfide bridge, and hence is easier to manipulate. The focus of the past year has been to complete the assignment of all possible proton, C-13, and N-15 resonances in the protein and the acquisition of experimental constraints in the form of those chemical shifts, dihedral angles from coupling constants, and inter-proton distances from nuclear Overhauser enhancements. That has now been accomplished and the upcoming year will focus on computations to utilize the experimental constraints to generate a family of three-dimension structures for the C74A target.

**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 two presentations at regional meetings. In the last year, Prof. Vincent became Co-editor-in Chief of the journal *Biological Trace Element Research*, published by Springer, and was made a fellow of the American College of Nutrition and a member of the editorial board of the journal *Polyhedron*. Prof. Vincent had one book and two peer-reviewed articles published; three peer-reviewed articles and two encyclopedia chapters were accepted for publication. Prof Vincent had continuing funding from NSF and AICHE and new funding from NSF and 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. Additionally, 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 one journal, 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 Feb. 3, 2015 review of citations on ISI Web of Science, Dr. Vincent had 121 publications identified (excluding abstracts, letters, corrections, etc.) that resulted in 7,476 citations, giving an average of 62 citations per publication. He has an H-index of 44. Dr. Vincent has one publication cited nearly 1400 times.

**Dr. 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. Initial experiments have shown some rectification; a manuscript describing this work in preparation. 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. Collaborations have been developed with Prof Timkovich (UA, NMR structural studies) and Profs Dom Qualley and Lindsey Davis (Berry College) on fluorescent nucleosides.

In service, Woski continues to serve as the Department of Chemistry's Director of Graduate Studies. Development of a new graduate core curriculum is underway. Furthermore, streamlining and electronic storage of graduate student records will be implemented shortly.

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 been renewed for another three years.

## **II. Staff Highlights**

**Staff Changes:** Ms. Jackie McPherson retired after long service to the Department as administrative secretary. Ms. April McIntosh was promoted to fill this position and Ms. Rachel Marcum was recently hired to replace Ms. McIntosh as an office associate.

## **III. Student Highlights**

Department students received recognition on campus and nationally for their academic and research success. The list of awards received by department graduate and undergraduate students is provided below.

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

#### **External Awards**

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

Melody Kelley (Blackstock)                      Carl Saint Louis (Blackstock)

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

Jordyn L. Johnson (Frantom)

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

Michelle L. Stover (Dixon)

##### **ACS Division of Organic Chemistry Graduate Research Symposium**

Ashley Jolly (Bonizzoni)

#### **University Awards**

##### **Graduate Council Fellowship**

Jack Albert (Snowden)                      Dalton Burks (Papish)

Garima Kumar (Frantom)

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

Joel Cassidy (Rupar)                      Tabitha Sutch (Szulczewski)

##### **McNair Graduate Fellowship**

Pandora E. White (Vincent)

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

Joseph Meany (Woski)—3<sup>rd</sup> place in University-wide competition

## **Chemistry Department Awards**

### **Outstanding Dissertation Award**

Parker McCrary (Rogers)

### **Outstanding Research by a Doctoral Student**

Caleb Hill (Pan)

### **Outstanding Graduate Student Award**

Michele Stover (Dixon)

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

Shengjie Zhang (Dixon)

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

Kerry Barnett (Shaughnessy)

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

Molly Lockhart

## **Undergraduate Student Awards**

### **External Awards**

#### **Southeastern Undergraduate Research Conference Awards**

Shuwen Yue (Dixon) – 1<sup>st</sup> place oral (Physical)

Megan Johnston (Shaughnessy) – 1<sup>st</sup> place oral (Organic/Inorganic)

Kathryn Adams (Bonizzoni) – 2<sup>nd</sup> place oral (Organic/Biochemistry)

Anthony Curto (Papish) – Poster award

Julia Murphy (Dixon) – Poster award

#### **Barry M. Goldwater Scholarship 2014-15**

Lynda Truong (Woski) 2014-15

Sarah McFann (Arduengo) 2015-16

### **University Awards**

#### **Randall Outstanding Undergraduate Research Awards**

Yuliya Birman (Frantom)

Erin N. West (Frantom)

Kyle C. Glisson (Bonizzoni)

Meredith Rickard (Dixon)

Sean Miller (Dixon)

Shuwen Yue (Dixon)

#### **Undergraduate Research and Creative Activity Conference**

Natural Science & Mathematics oral presentation

Shuwen Yue (Dixon): 2<sup>nd</sup> place

Ryan Hacherl (Cassady): 4<sup>th</sup> place

Sean Miller (Dixon): Honorable mention

Natural Science & Mathematics poster presentation

Kindle Williams (Woski): 3<sup>rd</sup> place

Lynda Truong (Woski): Honorable mention

**A&S Awards**

**Distinguished Undergraduate Scholars**

Marcus Hill Brakefield

**Michael T. Wilder Memorial Endowed Scholarship**

Olivia C. Roe

**Chemistry Department Awards**

**Outstanding Chemistry Undergraduate Student Award**

Yuliya Birman

Sean Miller

**Outstanding Chemistry Undergraduate Student Research Award**

Mary Katherine Kuykendall

Kindle Williams

**The American Institute of Chemists Award**

Meredith Rickard

Lynda Truong

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

Marcus Hill Brakefield

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

Lynda Truong

**Outstanding Analytical Chemistry Student Award**

Nicole Chambers

**Outstanding Organic Chemistry Students Award**

Katherine Baggett

Tu Minh Vo

Stephen McClain

Michelle Weyhaupt

**Outstanding Nursing Student Award**

Emily Chiaravalloti

**Outstanding General Chemistry Students Award**

William Baird

Larissa Magera

Blair Bush

Martin Schwarze

Shaun Hogan

Miranda White

Brennen Lummus

Olivia Willemsen

Kara Macintyre

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

Maya Nicolle Crawford	Calvin Daniel Muth
Samantha Lynn Dyroff	Amy E. Nealon
Stephen D. Emerson	Abigail Lynn Paulson
Jacqueline Rochelle Harris	Peyton Dees Presto
Jeremy Lane Hitt	Sarah E. Puckett
Amanda Kathleen Ivy	Alex L. Reeder
Alexis Leonora Holt Kentros	Trey H. Richardson
Elijah Patrick Kuhn	Kristen Nicole Sabino
Jordan Kristine Kurdi	Cody H. Savage
Mary Kaitlyn Kuykendall	Alexander B. Tankersley
William Shelby Layfield	Mackenzie L. Valentin
John A. Lundeen	Jacqueline M. Visina
Rachel Socorro Madey	Jacob C. Wilson
Tristan Marshall McGinnis	Wenzhi Yao
Madison Rebecca Monnette	Shuwen Yue

### IV. Faculty Research Productivity

**Publications and Presentations:** The productivity of the Chemistry faculty remained strong, although several metrics slipped from the previous year (Tables 1 and 2). The chemistry faculty published 115 peer-reviewed papers during this year. This value represents a drop from last year's total of 128, which was a 5-year high for the department, but is in line with the 5-year average. This corresponds to 4.4 publications per faculty member. Another 10 papers have been accepted, but had not been published as of March 31, 2015. The faculty submitted a total of 126 papers (4.8/faculty) during this FAR year, which includes papers that were also published in 2014-15. A total of 13 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 208 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
2014-15	115	23 (\$1.7 M)	75 (\$21 M)	54 (\$10.1 M)	\$2.63 M	208
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

<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 from OSP annual report.

**Contract and Grant Activity:** The Department faculty continue to effectively attract research dollars to the university despite the tough financial climate (Tables 1 and 3). Chemistry faculty submitted 75 proposals (61 proposal equivalents) with a total value of \$21 million. The

number of submissions is below the five-year average, but the requested dollars is similar to recent years. Faculty were awarded 23 contracts and grants (19 proposal equivalents) with a value of \$1.7 million. The awarded dollars represents a significant decrease from last year as well as the five-year average. The number of in-force awards (54) is down from last year as is the total amount of in-force funding (\$10 million). Research expenditures continued a four-year trend of declining. The challenge faced by faculty is that opportunities for submission of grant proposals are being limited at many agencies. For example, NSF has a single submission window for chemistry proposals. In addition, funding rates remain at historical lows. Faculty must continue to aggressively seek funding for all possible sources in the face of these negative trends in order for the department's research efforts to remain highly productive.

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

Faculty	Peer-Reviewed Publications			Books		Patents		Talks
	Sub	Acc	Pub	Book	Chap	App	Iss	
Arduengo	1	0	2	0	0	0	0	6
Bakker	6	0	5	0	0	1	0	7
Blackstock	0	0	0	0	0	1	0	0
Bonizzoni	2	0	3	0	0	0	0	24
Bowman	4	1	4	0	1	0	0	9
Busenlehner	0	0	0	0	0	0	0	0
Cassady	3	0	3	0	0	0	1	13
Dixon	19	0	21	0	0	0	0	18
Frantom	2	0	4	0	0	0	0	8
Goebbert	3	0	1	0	0	0	0	0
Gupta	19	4	12	0	0	0	0	20
Jennings	2	1	1	0	0	0	0	1
Metzger	2	0	1	0	0	0	0	3
Nikles	0	0	1	0	0	0	0	0
Pan	4	0	4	0	0	2	0	11
Papish	3	0	1	0	1	2	0	14
Rogers	34	0	34	0	0	7	6	42
Rupar	1	1	0	0	0	0	0	2
Shaughnessy	7	0	5	1	1	0	0	8
Snowden	1	0	2	0	0	0	0	2
Street	2	0	2	0	0	0	0	3
Szulczewski	6	0	6	0	0	0	0	2
Timkovich	0	0	0	0	0	0	0	0
Vaid	0	0	0	0	0	0	0	0
Vincent	5	3	3	1	0	0	0	8
Woski	0	0	0	0	0	0	0	7
<b>Total</b>	<b>115</b>	<b>10</b>	<b>126</b>	<b>2</b>	<b>3</b>	<b>13</b>	<b>7</b>	<b>208</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	16	\$2,317,989	3	\$20,782	0	\$20,782
Bakker	0	\$0	0	\$0	3	\$83,642
Blackstock	1	\$5,000	1	\$30,000	3	\$190,500
Bonizzoni	5	\$1,310,626	1	\$2,970	1	\$6,970
Bowman	1	\$546,161	1	\$234,000	1	\$300,874
Busenlehner	3	\$1,529,610	0	\$0	0	\$0
Cassady	3	\$1,224,125	0	\$0	2	\$575,830
Dixon	6	\$1,306,127	4	\$338,097	7	\$2,471,875
Frantom	0	\$0	2	\$305,891	2	\$1,009,418
Goebbert	3	\$1,443,920	0	\$0	2	\$8,100
Gupta	6	\$1,861,292	1	\$30,000	6	\$1,606,073
Jennings	2	\$858,079	0	\$0	0	\$0
Metzger	1	\$505,323	0	\$0	0	\$0
Nikles	5	\$739,446	0	\$0	2	\$39,575
Pan	5	\$2,020,133	0	\$0	3	\$902,202
Papish	5	\$1,215,631	1	\$37,500	1	\$178,401
Rogers	0	\$0	3	\$383,786	7	\$2,341,248
Rupar	3	\$1,587,785	0	\$0	1	\$47,760
Shaughnessy	0	\$0	2	\$40,171	3	\$720,205
Snowden	1	\$5,500	0	\$0	2	\$589,119
Street	1	\$404,210	1	\$8,403	2	\$185,103
Szulczewski	3	\$446,790	0	\$0	0	\$0
Timkovich	1	\$183,182	0	\$0	0	\$0
Vaid	0	\$0	0	\$0	0	\$0
Vincent	4	\$1,243,514	2	\$150,000	5	\$333,705
Woski	0	\$0	1	\$140,000	1	\$297,709
<b>Total</b>	<b>75</b>	<b>\$20,754,443</b>	<b>23</b>	<b>\$1,721,600</b>	<b>54</b>	<b>\$10,187,491</b>

<sup>a</sup>In-force C&G refer to grants in force on 3/31/14. 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 15,996 and 11,862 in the fall 2014 and spring 2015 semesters, respectively. The total of 27,721 SCH represents a 3.6% increase compared to 2013-14, which is the first single digit growth over the past 7 years. Table 4 shows the past five years of enrollment trends in Chemistry. The Department has seen a 52% increase in credit hour production from 2010-11 to 2014-15. The bulk of this growth has been at the undergraduate level, primarily in the service level courses. Student credit hours have grown 55% at the undergraduate level and 14% at the graduate over the past five years. The trend of significant growth in the department's service courses appears to be slowing, however, as the size of incoming classes begins to flatten out.

**Table 4. Total Credit Hour production**

Academic Year	Undergraduate	Graduate	Total	% Change
2014-2015	26,132	1,589	27,721	+3.6%
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%

Growth in student credit hour production has slowed, particularly for our service courses at the 100- and 200-level. Total credit hour production by semester for undergraduate courses is shown in Table 5. 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 growth in our service courses. The 100 level courses (101/102, 104/105, and 117/118) grew by 5% over last year and have grown by approximately 51% since 2010-11. After significant growth in organic chemistry in 2013-14, a small decrease in credit hour production occurred this year. This drop corresponds to a small growth in CH 102 in spring 2013. Enrollment in organic will probably again be flat in 2015-16 based on this year's CH 102 enrollment. Student credit hour production in the upper level chemistry courses (300-400 level) increased at a slower rate than the previous two years (8.6%). The continued strong growth reflects the recent growth in the number of chemistry majors, who are the main audience for our 300- and 400-level courses. In addition, our biochemistry course (CH 461) is a popular course for chemical engineering majors.

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

Academic Year	Fall Semester	Spring Semester	Total (% growth)
2014-2015	15,096	11,036	26,132 (3.8%)
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%)

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

Academic Year	100 Level	Organic	Upper (% growth)
2014-2015	19,772 (5%)	4,941 (-2%)	1,419 (8.7%)
2013-2014	18,824 (9%)	5,035 (31%)	1,306 (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%)

Graduate student credit hour production was essentially flat (-1%) after six years of continued growth. After several years of growth, our graduate student population has reached a steady state. Graduate student credit hours have increased by 14% since 2010-11.



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

Academic Year	Fall Semester	Spring Semester	Total
2014-2015	846	719	1,565 (-1%)
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%)

**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	27	24	51	68
Bakker	1,308	13	1,321	799	14	813	2,134
Blackstock	312	23	335	306	40	346	681
Bonizzoni	574	12	586	476	29	505	1,091
Bowman	133	16	149	0	18	18	167
Busenlehner	1	20	21				21
Cassady	240	18	258	2	50	52	310
Dixon	103	34	137	5	18	23	160
Frantom	224	55	279	36	47	83	362
Goebbert	286	20	306	38	32	70	376
Gupta	0	16	16	48	22	70	86
Jennings	13	46	59	550	17	567	626
Metzger	0	163	163	0	162	162	325
Nikles	856	10	866	849	6	855	1,721
Pan	4	57	61	208	20	228	289
Papish	59	41	100	2	10	12	112
Rogers	3	47	50	3	26	29	79
Rupar	3	39	42	846	23	869	911
Shaughnessy	647	19	666	479	29	508	1,174
Snowden	643	25	668	28	65	93	761
Street	577	18	595	1	25	26	621
Szulczewski	1,441	16	1,457	37	11	48	1,505
Timkovich	628	6	634	708	6	714	1,348
Vaid	852	6	858	719	4	723	1,581
Vincent	2	34	36	325	20	345	381
Woski	1,546	94	1,640	152	42	194	1,834
Total	10,461	859	11,320	6,644	760	7,404	18,724
Average	402	33	435	256	29	285	720
Median	232	20	269	43	23	128	501

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 2014-15 academic year. For the fall semester, Chemistry TT faculty averaged 435 SCH (median 269). For the academic year, the departmental average was 720 student credit hours per faculty over the two-semester period while the median production was 501 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 nearly 4,000 SCH this year. In addition, a total of 8 PTTI lines were used during the academic year. Part-time instructors generated over 5,000 SCH in the department this year. After decreasing our reliance on PTTI lines during the 2012-13 academic year, continued student growth has resulted in the continued need for 8 PTTI lines/year.

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

Faculty	Rank	Fall SCH	Spring SCH	Total SCH
Leung	CLTF	2,096	1,802	3,898
Cojocar	PTTI (4 classes)	1,108	1,496	2,604
McDuffie	PTTI (4 classes)	1,472	1,160	2,632
Total		4,676	4,458	9,134

The number of students declaring chemistry as their major in the spring semester of 2015 was 253, up 23% from the spring of 2014 (Table 10). The number of majors in Chemistry has grown significantly over the past three years after several years of little change in the number of majors. Since fall 2010, the number of fall chemistry majors has grown from 144 to 259 (+78%). 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 as a result of the increased number of majors.

**Table 10. Undergraduate Chemistry Major Trends**

Year	Fall	Spring
2014-15	259	253
2013-14	192	206
2012-13	156	181
2011-12	157	138
2010-11	144	119

During the calendar year of 2014, the Chemistry Department graduated 27 students (Table 11). This represents an increase over the 2013 calendar year. Of particular note, 40% 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 (20/27) graduated with distinction (*cum laude* or higher). We can anticipate continued strong degree production next year as 27 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>2014</b>	Pre-Health	15	0	1	16
	ChE/CH	0	0	1	1
	ACS	10	0	0	10
	<b>Total</b>	<b>25</b>	<b>0</b>	<b>2</b>	<b>27</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>

### **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, 2014 to March 31, 2015 compared to previous years are given below in Tables 12-16. Graduate enrollment in fall 2015 decreased to 90 doctoral+masters students, which is an average of 3.7 students/tenured or tenure-track faculty. Enrollment of females, who are underrepresented in chemistry, remains strong with 43% (39/90) of the overall graduate population and 47% (28/60) of the domestic student population being female. Underrepresented racial groups continued to be strongly represented with African-Americans/Native-Americans/Pacific Islanders comprising 18.3% (11/60) of domestic graduate student population. The graduate student population continues to hold with clear majority of domestic students versus international students (67% vs. 33%).

**Table 12. Graduate Student Enrollment Trends**

<b>Year</b>	<b>Total Students</b>	<b>Ph.D.</b>	<b>M.S.</b>	<b>PLA (Ph.D.)</b>	<b>Postdocs</b>
<b>Fall 2014</b>	<b>90</b>	<b>88</b>	<b>2</b>	<b>0</b>	<b>12</b>
Fall 2013	97	95	2	0	15
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.**

<b>Year</b>	<b>USA</b>	<b>Foreign</b>
<b>Fall 2014</b>	<b>60</b>	<b>30</b>
Fall 2013	65	32
Fall 2012	65	29
Fall 2011	66	27
Fall 2010	61	22
Fall 2009	49	28

**Table 14. Nationality Distribution.**

<b>Year</b>	<b>USA</b>	<b>China</b>	<b>India</b>	<b>Eastern Europe</b>	<b>Other South/East Asia</b>	<b>Other</b>
<b>Fall 2014</b>	<b>60</b>	<b>16</b>	<b>2</b>	<b>1</b>	<b>2</b>	<b>9</b>
Fall 2013	65	19	4	1	2	6
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.**

<b>Year</b>	<b>Total</b>	<b>Male</b>	<b>Female</b>
<b>Fall 2014</b>	<b>90</b>	<b>51</b>	<b>39</b>
Fall 2013	97	58	39
Fall 2012	94	56	38
Fall 2011	94	55	39
Fall 2010	83	47	36
Fall 2009	77	42	35

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

<b>Year</b>	<b>Male</b>	<b>Female</b>	<b>African-American</b>	<b>Hispanic</b>	<b>Native-American</b>	<b>Pacific-Islander</b>
<b>Fall 2014</b>	<b>32</b>	<b>28</b>	<b>8</b>	<b>0</b>	<b>1</b>	<b>2</b>
Fall 2013	37	28	11	1	1	
Fall 2012	39	26	10	1	1	
Fall 2011	39	27	11	0	1	
Fall 2010	36	26	10	1	0	
Fall 2009	29	20	7	1	0	

A snapshot of the methods of supporting our graduate student population for fall 2015 is shown in Table 17. The number of TAs allotted to fulfill our teaching mission has increased to 59 TAs for AY 2014-15, 9 of which are soft money TAs. We purposefully oversubscribed by 2.66 TA lines in fall 2014. This overage was partly recovered in spring 2015 when we employed 57.22 TAs. We expect the budget to balance with the summer appointments. With enrollment increases projected to continue, the addition of 12 soft TA to our 50 “hard” lines will hopefully meet our fall 2015 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 2014-15 are shown below, along with those from several previous years. For this academic year, the chemistry department had 5 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 & SREB. The end of the GAANN funding after AY 2012 was responsible for the decrease in external fellowships in the current year. We reapplied for this grant in May 2015.

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

Year	TA	RA	Staff	External Fellowship	Internal Fellowship	Department	Self Support
<b>Fall 2014</b>	<b>61.66</b>	<b>15.66</b>	<b>0</b>	<b>2</b>	<b>5</b>	<b>0</b>	<b>7.66</b>
Fall 2013	60.50	22.16	0	6	3	0	6
Fall 2012	47.00	27.66	0	13	4	0	5
Fall 2011	45.66	27.33	0	11	3	0	8
Fall 2010	40.83	25.83	0	10	5	0	3
Fall 2009	37.66	29.33	0	3	5	0	4
Fall 2008	36.00	24.33	0	6	4	0	4
Fall 2007	30.33	34.33	0	2	3	0	5
Fall 2006	28.33	36.66	1	4		0	2

**Support breakdown: TAs: 61.66** = 13.0 first-year students, 13.88 second-year students, 34.78 third-year and beyond. **RAs: 15.66** = 0 first-year students, 2.00 second-year students, 13.66 third-year and beyond. **Fellowships:** 3 GCF (D. Burks, J. Albert, G. Kumar), 1 NAA (T. Sutch), McNair (P. White), 1 NSF (J. Johnson), 1 SREB (C. Saint-Louis).

A total of 30 students received graduate degrees from the department last year (16 MS and 14 PhD). It is anticipated that the number of doctoral graduates will increase in the coming year.

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

Calendar Year	MS	PhD	Total
<b>2014</b>	<b>16</b>	<b>14</b>	<b>30</b>
2013	10	10	20
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. 2014-2015 PhD degrees**

December 2014	Spring 2015	Summer 2015 (anticipated)
Ashley Casey	Ed Ellingsworth	Michele Stover
Changgeng Feng	Adam Magyar	Gregory Dye
Amanda Glover	Tanya Mikulas	Ashley Jolly
Caleb Hill	Katrina Staggemeier	Alex Cruce
Melody Kelley		Zhexi Li
		Chris Griggs
		Jue Wang

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

A total of thirteen (13) students entered our graduate program in AY 14/15. This class was supported by 12 full or partial graduate teaching assistantships (TAs) and two fellowships. This class included six females and seven males. Ten of these students were US citizens and three were foreign nationals.

A fall 2014 incoming class of sixteen (16) students is currently committed, with several more likely. The entering class (as is) will be supported by fifteen full or partial TAs, and partially supported by two National Alumni fellowships and one McNair Scholarship. One student will also hold a Dean's Diversity Award supplement. None of the incoming students has a Graduate Council Fellowship; the Department secured four for its nominees, but none of these students accepted our offer.

Our graduate TA stipend (also usual for RAs) of \$23,928, with no-cost health coverage, for AY 2014-15 is competitive with schools in the Southeast as determined from the recent SE Chair's Survey. Net regional stipends range from \$19,000-27,000. Our stipend will likely need to be increased again in the future, especially as fees (such as credit hour fees) begin to degrade their value. 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). More of these kinds of offers might become available should we be awarded GAANN (Graduate Assistantships in Areas of National Need) funding in the current competition. 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 sixteen students currently admitted for fall 2015 have an average GRE score of 307 and 3.4 GPA, and three are conditional admission. These scores are consistent with our recently established average values. One student received a Dean's Diversity award and accepted our admissions offer. Four of our nominated students were awarded Graduate Council Fellowships but none 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
<b>F 15*</b>	<b>16</b>	<b>13</b>	<b>3</b>	<b>0</b>	<b>12</b>	<b>4</b>	<b>307</b>	<b>82</b>
Sp 15	1	1	0	0	1	0	313	
F 14	15		2	0	11	4	309	N/A <sup>@</sup>
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 @-All foreign students had English language or US-based degrees.

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

Year	USA	China & Taiwan	India	Eastern Europe	Korea & Thailand	Others
F 15*	13	1	1	0	0	1
AY 14/15	12	2	0	0	0	2 (Canada)
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>		
	<b>Total</b>	<b>M</b>	<b>F</b>	<b>Total</b>	<b>M</b>	<b>F</b>	<b>African-American</b>	<b>Hispanic</b>	<b>Native-American/PI</b>
F15*	16	7	9	3	2	1	1	0	0
AY 14/15	12	7	5	4	1	3	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>**

<b>Year</b>	<b>Offers Made</b>	<b>Offers Accepted</b>	<b>Success Rate</b>	<b>Domestic Success Rate</b>	<b>Foreign Success Rate</b>
F15*	31	16	52%	13/24 = 54%	3/6 = 50%
AY 14/15	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 is up significantly: 74 applications, including fifteen (15) from Alabama. This may reflect real improvement in our regional recruiting generally or our efforts specific to this year (see below). Our number of international applications, which was on the order of 150 per AY over the past decade, is now much lower (54 international applications for fall 2015). 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, and Gupta) from these applicants.

The incoming fall 2015 class, as it stands, does appear to be reasonably diverse. Women, who had been traditionally underrepresented in our discipline, account for 9/16 of the class (the Dean's office (A&S) has ruled 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 African American woman admitted for fall has accepted and will receive a Dean's Diversity Award.

We have been involved in a variety of recruiting efforts. Prof. Papish organized and chaired the Southeastern Undergraduate Research Conference (SURC) hosted by our Department here in Shelby Hall on 7 February 2015. This very successful meeting brought more than fifty active undergraduate researchers from seventeen regional programs to UA. Prof. Oleg Ozerov of Texas A&M University was keynote speaker. Eight university chemistry programs, other than UA, sent recruiters to the event. Because registration fees are charged, hosting SURC is essentially cost-free, aside from time and effort. Unfortunately we cannot host more often as the event rotates through a number of regional departments.

Prof. Frantom led the planning and execution of our Department's first ever graduate recruiting weekend. From 27-29 February 2015 we hosted fifteen prospective graduate students in Tuscaloosa. While here they had the opportunity to meet with our graduate students and faculty, tour the facilities of the Department and The University, and sample the campus lifestyle. We made offers to fourteen of these students, and ultimately nine of these accepted and are part of the fall 2015 class (64% success rate). Simple cost accounting suggests that this approach is not significantly more expensive than the individual visits we have historically supported on a per person basis. We believe the evidence of the results and feedback from both the invitees and our faculty indicate the recruiting weekend is a useful approach and should be used when the anticipated size of the recruiting class warrants the effort.

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 other domestic applicants for individual visits to the Department. We paid approximately \$1600 in application fees, mostly for domestic applicants. The department supported at least four other recruiting trips for faculty visits to other departments regionally and nationally.

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

The Department continues 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 for the second time in collaboration with Dr. Vincent Scalfani from UA Libraries in fall 2014.

Stemming from the department's graduate program "retreat" in December 2013 we are beginning 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 2014-15 academic year are shown below in Tables 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 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. Cassidy (MS), and Dr. Papish (X-ray) supervise our major instrument facilities. Each plays a key role in ensuring this shared instrumentation remains in working conditions. Drs. Street (NOBCChE), Woski (CGSO), Blackstock (SCACS), and Shaughnessy (GSE) serve as advisors to departmental student groups.

**Table 26. Standing Department Committees 2014-15**

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<b>Executive Committee</b> K. Shaughnessy (Chair) S. Woski S. Street M. Jennings 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) J. Vincent R. Timkovich G. Szulczewski D. Dixon S. Blackstock D. Leung
<b>Graduate</b> S. Woski (Chair) P. Rupar 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	<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 S. Pan E. Papish R. Rogers	T. Snowden S. Street G. Szulczewski R. Timkovich J. Vincent S. Woski
<b>REU Committee</b> J. Vincent (Chair) S. Woski K. Shaughnessy C. Cassady G. Szulczewski		<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: E. Papish

**Table 27. Special Committees for 2014-15**

<b>Materials Chemistry Search Committee</b>	<b>Chemical Biology Search Committee</b>
S. Street (Chair)	S. Woski (Chair)
A. Gupta	L. Busenlehner
S. Pan	P. Frantom
E. Papish	M. Bowman
R. Sidje (A&S)	M. Johnson (Biology)

**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), College Leadership Board Faculty Representative (Cassady), Technology and Research Working Group (Dixon), A&S Scholarship Committee (Jennings), Diversity Committee (Leung), Committee for Undergraduate Research and Creative Activity (Pan), A&S Tenure and Promotion Committee (Snowden), Math Department Chair Search Committee (Shaughnessy), Pre-Health Professions Advisory Committee (Shaughnessy), Undergraduate Curriculum Committee (Vincent), College Academy for Creative and Scholarly Activity Committee (Vincent). 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: QEP Implementation Committee (Blackstock), Technology and Learning Committee (Bonizzoni), Association of Women in Science Advisor (Cassady), Laboratory Safety Committee (Cassady), Burnum Award Committee (Dixon), CBHP Admissions Committee (Dixon), Technology Research Advisory Committee (Dixon), Student Health Committee (Goebbert), Conflict of Interest Policy Committee (Gupta), MINT Faculty Search Committee (Gupta, Szulczewski), CAF Users Advisory Committee (Nikles, Chair; Szulczewski), Intellectual Property Committee (Nikles), SACS Graduate Committee (Shaughnessy), Alabama Boxing Club Faculty Advisor (Street), Campus Laser Safety Committee (Street, Chair), Outdoor Adventure Club Advisor (Street), Tri-Campus Materials Science Program Exam Committee (Street), RGC (Street, Area A Chair), University Ombudsperson (Street), Academic Classroom Committee (Szulczewski), Institutional Animal Care and Use Facility (Vincent, Vice-Chair), and Laboratory Safety Committee (Vincent, chair).

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 senator. Dr. Vincent is on the Faculty Senate Steering, Faculty Participation in the Selection of Deans and Department Chairpersons and Evaluation of Academic Programs, and Academic Affairs (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. 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. Chemistry faculty served as judges for the UA Undergraduate Research and Creative Activity Conference (Rupar, Snowden, Shaughnessy) and 3MT competition (Shaughnessy). 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), 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, Bonizzoni), the U. Chicago Center for EPR Imaging (Bowman), ALCF User Advisory Committee, Argonne National Lab (Dixon), Oak Ridge National Lab OLCF User Advisory Committee (Dixon), User Executive Committee, William R. Wiley Environmental Molecular Science (Dixon), External Advisory Board of NSF Sponsored Center for Mathematical Achievement in Science & Technology at Grambling State University (Nikles). A number of department faculty serve on editorial or advisory boards to scientific journals including: *Applied Magnetic Resonance* (Bowman), *Journal of Magnetic Resonance* (Bowman), *Spin Physics*, *Spin Chemistry*, and *Spin Technology* (Bowman), *International Journal of High Performance Computing* (Dixon), *Journal of Physical Chemistry* (Dixon), *Journal of Fluorine Chemistry* (Dixon), *International Journal of Supercomputer Applications* (Dixon), *Computational and Theoretical Chemistry* (Dixon), *Metallurgical and Materials Transaction* (Gupta), *Rare Metals* (Gupta), *Nature Scientific Reports* (Gupta), *Advances in Physical Chemistry* (Metzger), *The Chemical Record* (Metzger), *Journal of Biomedicine and Biotechnology* (Vincent), *Polyhedron* (Vincent), *F1000 Research* (Woski). Dr. Vincent is co-editor in chief of *Biological Trace Element Research*.

**Professional Organizations:** Department faculty serve on committees for a range of professional science and education organizations: Executive Committee, ACS Division of Fluorine Chemistry (Dixon), ACS Committee on Publications (Dixon), ACS Councilor for Division of Fluorine Chemistry (Dixon), ACS Committee on Publications (Dixon), American Chemical Society Polymer Examination Committee (Nikles), 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 500 manuscripts, 4 books or book chapters, and 300 grant proposals or preproposals. Faculty served on 8 grant panels during the year.

**Professional Meetings:** The Department hosted two regional professional meetings during this academic year. Dr. Michael Bowman and Dr. Lowell Kispert organized the Southeastern Magnetic Resonance Conference at UA in October. This meeting brought over 100 participants to the UA campus, including international visitors. In February, the Department hosted the Southeastern Undergraduate Research Conference (SURC). Dr. Elizabeth Papish led

organization of the SURC. Over 100 students and faculty from regional colleges and universities attended the conference. Dr. Dixon served so co-organizer for the 22<sup>nd</sup> Winter Organic Fluorine Conference. Dr. Cassidy served as the program committee organizer for the oral session at the American Society for Mass Spectrometry national meeting. Dr. Vincent served on the Scientific Committee of the 8<sup>th</sup> Conference on Metal Toxicity and Carcinogenesis. Dr. Nikles serves on the organizing committee for the NanoBio Summit meetings. The following department faculty organized symposia at national and international meetings: Dixon (2), Shaughnessy (1).

## 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 2014, 10 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 250 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.

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 2014. 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.

Noyce Program Summer Internship: Dr. Shaughnessy was a co-organizer of the Noyce program summer internship in 2014. The Noyce program is an NSF-funded grant at UA to increase the production of highly qualified secondary teachers in the areas of math, chemistry, and physics. The summer internship involved 15 students from UA and regional community colleges. The interns were exposed to scientific research on campus, learned about opportunities for high school teachers, and participated in teaching activities with middle school students.

High School Visits to UA: Dr. Bakker hosted the AP Chemistry classes from Hillcrest. 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. Dr. Jennings and Lisa Cox hosted a field trip by students from American Christian Academy to visit the chemistry glassblowing shop and other sites on campus. The Gamma Sigma Epsilon honorary society hosted an AP chemistry day. Students from local schools participated in hands on lab experiments, toured campus, attended a poster session by undergraduate researchers, and participated in chemistry Jeopardy.

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

As chair, I am working to more regular publish a department newsletter. This is part of an effort to better connect with our alumni and hopefully increase donations to the department support funds. The next newsletter will be distributed this summer. We hope to establish a twice-yearly schedule for distributing the newsletter.