Department of Chemistry
Mission Statement

The Department of Chemistry occupies a central position in the instructional, research, and outreach missions of the College of Science. Our courses provide the chemical foundation of science and engineering curricula of all colleges in the University. These courses broaden the students’ understanding of the structure and properties of matter. Our undergraduate and graduate degree programs prepare students for careers in chemistry and related disciplines. Our faculty’s research and scholarship generate and disseminate knowledge to the Commonwealth, our nation, and the world. Through outreach programs, the Department frequently shares this knowledge with practicing professionals and with primary and secondary school children.

To achieve our mission, the Department will continue to pursue multi-disciplinary research within the University, to innovate in the instruction of students, to forge partnerships with industry and government, and to establish a program in the chemical sciences of the highest rank.

The efforts of Laurie Good, Patricia Amateis, Brian Tissue, Gordon Yee, Paul Deck, Tom Bell, Hervé Marand, and EMillie Shephard in preparing, printing, and distributing this report are acknowledged and appreciated.

JMT, July 3, 2012
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EXECUTIVE SUMMARY

Learning: Undergraduate. Our undergraduate program remains strong. Faculty commitment to our majors classes (lecture and lab) is enthusiastic, and senior exit interviews confirm that our students value and appreciate their experience. Indeed, it might be argued that because of the quality of the experience and close interactions that our students have with their professors, chemistry majors at Virginia Tech enjoy a small school experience at a very large university. The total number of chemistry majors is holding constant, although the number of students graduating with a BA/BS in chemistry this past year was more in line with previous years (64, as opposed to the all time high of 89 in 2010 – 2011).

The Department’s major reinvestment in undergraduate education continues, buoyed by the introduction of lab fees, loans from the College of Science, and a unique partnership with Agilent Technologies. Both chemistry majors and the much larger group of non-majors who enroll in our service classes will have direct, hands-on experience with a variety of new instrumentation including GC/MS, NMR, UV/Vis, fluorimeters, atomic absorption spectrometers, a powder X-ray diffractometer, a flash calorimeter, and more. In the non-majors general chemistry laboratory, an entirely new set of experiments will be implemented to take advantage of this new equipment. A fringe benefit of this major investment is that it has reinvigorated the enthusiasm of the faculty, staff, and TAs who are associated with these courses.

Non-majors general chemistry, our largest service course, has struggled with teaching large numbers of students—sometimes with temporary faculty members—which made it difficult to maintain consistent content and standards among the various sections. The program is moving towards a more uniform and more rigorous experience for all students, a process that began with online homework, continues with the development of an “Instructors Manual,” and that by 2014 will culminate with common time/common content examinations. Coupled to the upgrade in the laboratory experience, our general chemistry offering will become a highlight of the first year experience for VT freshman.

Learning: Graduate. The Chemistry Department’s graduate program offers state-of-the art classes (taught by enthusiastic and dedicated faculty), research opportunities that range from studying the fundamental properties of molecules to addressing some of society’s biggest problems—and a well-funded, internationally-recognized faculty that mentor their students to prepare them for successful, satisfying and productive careers. Probably no better evidence for this statement is provided by the election of one of our alums (Joseph DeSimone) to the National Academy of Sciences this year.

The success of our Department, nearly 200 published peer-reviewed papers in top journals with most co-authored by graduate students, provides testimony to the fact that our research provides an outstanding platform for students earning an advanced research degree in chemistry. In addition to classes and research, our degree requirements focus on developing critical thinking skills, communication skills (written and oral), and creativity. With input from the faculty, the Graduate Education Committee continues to evaluate and re-evaluate the program and its requirements, introducing changes when necessary to enhance the quality of education for our students.

Discovery. With an impressive number peer-reviewed papers published this past year in top-tier journals, 150 published abstracts, preprints, and conference proceedings, on the order of 200 invited lectures and seminar presentations, and countless poster presentations delivered by faculty and students, this Department continues to build upon a long and stellar tradition of discovery. With the weakened economy, the end of the federal stimulus program (as well as and other factors), total research funding is down nationally in chemistry—a trend from which we were not spared. In short, competition for a diminishing funding pool is increasing. Nonetheless, our faculty remain successful in attracting funding that ranges from large, multiple-investigator to single-PI grants. Locally, nationally, and internationally, our faculty continues to be recognized with prestigious awards for the quality of their research.
Engagement. Faculty and staff in chemistry continued their active engagement in notable leadership, service, and outreach for the profession, University, and community. Most notably, at the time of this report, Virginia Tech was hosting the 2012 IUPAC (International Union of Pure and Applied Chemistry) World Polymer Conference—a tribute to the faculty members of this department who have made our polymer program one of the best in the world. In terms of service, faculty members in chemistry have taken on major leadership roles in the University that will profoundly shape our future, and nationally that will increase the recognition and prestige of our department. The K-12 outreach and education initiatives of our faculty continue to influence and motivate the next generation of scientists.

Diversity. For three years in a row, a member of the chemistry faculty has been the recipient of the College of Science Diversity Award: Judy Riffle (2010), Diego Troya (2011), and most recently, Felicia Etzkorn (2012). Gender diversity among the faculty ranks is improving and approaching the (admittedly low) average in chemistry; among our students, gender diversity is much more reflective of the overall population. Despite our best efforts, the recruitment of underrepresented minorities remains problematic both in terms of faculty and graduate students.

Challenges for 2012 – 2013 (and beyond). In preparation for the renovation of Davidson Hall (which began in early 2012), the entire building was evacuated. In Summer 2011, several research groups moved from Davidson Hall, or in some cases from Hahn Hall South, to the Corporate Research Center (CRC) located approximately three miles from campus. The Department of Biochemistry graciously made lab space available to faculty members in Engel Hall. The Department’s main office, and the computational research groups were moved to Hahn Hall North. Many faculty offices and our electronics shop were moved to the Surge Building. These relocations, though accomplished with remarkable efficiency and goodwill, unquestionably disrupted the research activities of the groups involved. Though Blacksburg Transit offers excellent service to and from the CRC during the academic year, that service is seriously curtailed during the summer months—and this imposes hardships on the affected students.

During this renovation period, the Department is seriously short of space, with several labs and offices overcrowded. The Davidson closure also resulted in the loss of classroom space, and the scattering of faculty and graduate students across the campus and beyond means that people must now travel further to teach their labs and classes. And, in many cases, the alternative classroom space was sub-par (e.g., large classes in the Graduate Life Center, where lighting is poor, and the chairs do not have desks.)

Many of these problems will vanish once Phase 1 of the renovation is complete and Davidson reopens. However, with the timing of Phase 2 (which will renovate the front end of Davidson) uncertain, the Department will likely face another set of disruptive moves.

Financially, there are drains on the department budget that may impact our ability to hire tenure track faculty in the next academic year (or more to the point—offer a startup package that is competitive). In addition to the debt incurred by the chemistry stockroom between 1999 – 2003 (which is now being addressed), the department was saddled with nearly $70K of additional debt because private research sponsors failed to follow through with payment for services provided. (It should be noted that the total
default was much larger; part of the debt was shared with the College of Science, and the bulk was borne by the Office of Sponsored Programs).

**Goals for 2011 – 2012: Status report.** In last year’s annual report, one of our major goals was to maintain, with minimal disruption, our high standards of instruction, research, and erudition during the complex process of relocating faculty, staff, students, teaching labs, research facilities, etc. during the Davidson renovation. In this context, the Department was enormously successful as evidenced by the activities summarized in this report. The collegiality and cohesiveness of the Department’s faculty and staff remain strong.

Another goal was to initiate faculty searches in macromolecular/polymer chemistry and drug discovery. Only the polymer search was approved, and the Department was successful in hiring Dr. John Matson, who will join the faculty in Fall 2012.

The Executive Committee continues to work on a departmental strategic plan that includes not only a hiring plan, but also clearly articulates our goals and the challenges we face in research, teaching, and outreach. The Department will continue to chart a course that will not only enable it to weather challenges, but allow it to improve in all areas of its mission with the long-term goal of becoming a top-ranked department nationally.

**Goals for 2012 – 2013.** A formal review of the Chemistry Department is long overdue—the last “five year review” was conducted in 1999. The Executive Committee has been charged with the responsibility of recommending to the Dean of the College of Science, individuals who will a) serve on the review committee from our faculty and VT community, and b) serve as external reviewers. The objective is to conduct that review during the 2012 – 2013 academic year. The Executive Committee will also need to complete the departmental strategic plan.

The Department hopes to submit a formal request to initiate a faculty search in the area of drug discovery and/or computation/theory, consistent with our hiring plan—assuming sufficient resources become available, and that VT is not facing a hiring freeze.

The Department needs to continue, and successfully complete, the search for two permanent instructors to cover teaching obligations in general chemistry and physical/analytical chemistry.

The Department will continue the phase-in of lab fees with our 2000-level labs, and begin planning for those at the 3000-level. In addition to its efforts directed towards enhancing general chemistry lecture and labs, the Undergraduate Committee will conduct a comprehensive, across the board assessment of laboratory courses for chemistry majors.

The Graduate Education Committee will make recommendations to the faculty pertaining to changes in the graduate curriculum that may: 1) Eliminate divisional course requirements to allow more flexibility, 2) eliminate the “reader system” for the literature review requirement, and 3) modify the original research proposal requirement so that it is separated from the third year review and no longer handled by the PhD advisory committee.
LEARNING: UNDERGRADUATE PROGRAMS

Overview

The undergraduate program continues to evolve in response to changing demands and opportunities. The long-term plan for general chemistry calls for common-time, common-content midterm and final examinations. The University registrar has agreed to work with the department to effect this change, which will involve the simultaneous use of almost every large classroom on campus four nights during the semester and final exam week. Dr. Cindy Cribbs has also started to write a manual to be provided to all general chemistry faculty to help to coordinate this effort. For instance, a fairly precise timeline of the presentation of topics will be created, one that includes which topics can be skipped and which are of greater importance. It will also provide a blueprint for hour examinations and navigating the grading system.

The search for an instructor to teach general chemistry this Spring brought three candidates to campus (out of roughly 50 applicants). We had hoped to find someone with at least a semester of lecturing experience. We made one offer and it was declined, so we will be short-staffed this coming year. It is our intention to continue this search in the Fall.

The initiation of a laboratory course fee for general chemistry created new opportunities for introducing instrumentation into the labs. Ms. Vicki Long has been assigned the task of renovating the experiments to incorporate the new equipment such as the gas chromatograph/mass spectrometers. This source of funding will also allow us to replace equipment on a 10-year schedule. Prior to this, there was no plan for replacing obsolete equipment purchased when the building was first opened. Course fees for other labs led to other improvements, including the purchase of a 400 MHz NMR for use by undergraduates.

We have shifted our summer school strategy to give teaching opportunities to our alums and very advanced graduate students, rather than hiring temporary faculty from nearby colleges. This change has been accompanied by more structured mentoring of these novice instructors. For instance, currently, Dr. Furong Sun, a recent PhD graduate, is teaching CHEM 1035, and Mr. Alec Wagner, an MS graduate, is teaching 1036. Ms. Lesley Owens (PhD expected Fall 2012) is teaching 2114 and 2124, analytical chemistry. The goal of this shift is to give first teaching experiences to our students who intend to enter the teaching profession so that they can feature this experience in their resumes.

At the upper division level, increasing enrollments (~250) necessitated the opening of a second section of the first semester of physical chemistry for life sciences (CHEM 4615). Because of a shortage of qualified teachers, Prof. Troya taught this second section as an overload. Projected demographics suggest that we will continue to need to teach this additional section.

The retirement of Mike Johnson, an instructor, is proving to be somewhat of a hardship for us, though perhaps an opportunity as well. Mike taught PChem I lab both Fall, Spring and Summer and Analytical lab. We searched for his replacement this Spring and were unable to find a suitable candidate. The plan is to re-open the search in the Fall. We hope to hire an experienced PhD level person who could also teach CHEM 4615 (PChem for life sciences), which would address the problem discussed above. In the near term, a second tenure-track faculty member will teach the added section of 4615.
As a result of the creation of the Integrated Science Curriculum (ISC) in the College of Science, we are losing two faculty-semesters. ISC Profs. Tim Long and Gary Long will each teach one semester as part of ISC. This will make it more difficult to cover our courses and probably necessitate the hiring of additional instructors. Prof. Tissue will be taking over Instrumental Analysis, CHEM 4114.

As shown in the table below, our enrollment numbers have been steady for the past three years, with a shift towards more secondary chemistry majors. This probably reflects more BA students (double majoring) and is consistent with the increased enrollment in PChem for life sciences the past year or two. The number of chemistry minors is likely decreased because the requirements for the minor have become more rigorous and now include a semester of PChem.

### Departmental Enrollment Trends

<table>
<thead>
<tr>
<th></th>
<th>Fall 03</th>
<th>Fall 04</th>
<th>Fall 05</th>
<th>Fall 06</th>
<th>Fall 07</th>
<th>Fall 08</th>
<th>Fall 09</th>
<th>Fall 10</th>
<th>Fall 11</th>
</tr>
</thead>
<tbody>
<tr>
<td>Primary CHEM majors</td>
<td>164</td>
<td>157</td>
<td>190</td>
<td>213</td>
<td>239</td>
<td>258</td>
<td>285</td>
<td>284</td>
<td>259</td>
</tr>
<tr>
<td>Secondary CHEM majors</td>
<td>48</td>
<td>45</td>
<td>45</td>
<td>45</td>
<td>49</td>
<td>61</td>
<td>70</td>
<td>64</td>
<td>90</td>
</tr>
<tr>
<td>TOTAL CHEM majors</td>
<td>212</td>
<td>202</td>
<td>235</td>
<td>258</td>
<td>288</td>
<td>319</td>
<td>355</td>
<td>348</td>
<td>349</td>
</tr>
<tr>
<td>CHEM minors</td>
<td>312</td>
<td>293</td>
<td>272</td>
<td>354</td>
<td>481</td>
<td>562</td>
<td>677</td>
<td>768</td>
<td>641</td>
</tr>
</tbody>
</table>

### Chemistry Graduates (BA/BS); Demographics

<table>
<thead>
<tr>
<th></th>
<th>Fall 09/Spring 10</th>
<th>Fall 10/Spring 2011</th>
<th>Fall 11/Spring 2012</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Graduates</td>
<td>60: 36 BA, 24 BS</td>
<td>89: 56 BA, 33 BS</td>
<td>64: 39 BA, 25 BS</td>
</tr>
<tr>
<td>Female</td>
<td>27</td>
<td>40</td>
<td>31</td>
</tr>
<tr>
<td>Male</td>
<td>33</td>
<td>49</td>
<td>33</td>
</tr>
<tr>
<td>Summa Cum Laude</td>
<td>3</td>
<td>4</td>
<td>8</td>
</tr>
<tr>
<td>Magna Cum Laude</td>
<td>8</td>
<td>8</td>
<td>6</td>
</tr>
<tr>
<td>Cum Laude</td>
<td>2</td>
<td>6</td>
<td>7</td>
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<tr>
<td>Honors Scholar</td>
<td>1</td>
<td>5</td>
<td>5</td>
</tr>
<tr>
<td>Honors Program In-Honors</td>
<td>2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Honors Baccalaureate</td>
<td></td>
<td></td>
<td>2</td>
</tr>
<tr>
<td>Honors Program Commonwealth Scholar</td>
<td>1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Honors Scholar in Health Studies</td>
<td>1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Enrollment data for our service courses are provided in the following table.

Also related to service course enrollments is the fact that Hervé Marand has developed an on-line version of CHEM 4615 Physical Chemistry for the Life Sciences for fully asynchronous teaching with funding from the Enterprise Fund (Office of the Provost). The development of this course is motivated by the fact that Life Science students often take Physical Chemistry courses in their senior year. Unfortunately, a large number of them do not pass this class at their first attempt. Hence, offering this class twice a year would be a great benefit to a large number of students.
### Fall 2011 and Spring 2012 Enrollments in our Service Courses (i.e., for non-majors)

<table>
<thead>
<tr>
<th>COURSE</th>
<th>Fall 2011</th>
<th>Spring 2012</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intro to Chem</td>
<td>CHEM 1015</td>
<td>348</td>
</tr>
<tr>
<td>Intro to Chem 2nd semester</td>
<td>CHEM 1016</td>
<td>315</td>
</tr>
<tr>
<td>Intro to Chem lab</td>
<td>CHEM 1025</td>
<td>80</td>
</tr>
<tr>
<td>Intro to Chem lab 2</td>
<td>CHEM 1026</td>
<td>44</td>
</tr>
<tr>
<td>Gen Chem</td>
<td>CHEM 1035</td>
<td>3047</td>
</tr>
<tr>
<td>Gen Chem 2</td>
<td>CHEM 1036</td>
<td>0</td>
</tr>
<tr>
<td>Gen Chem lab</td>
<td>CHEM 1045</td>
<td>2267</td>
</tr>
<tr>
<td>Gen Chem lab 2</td>
<td>CHEM 1046</td>
<td>1115</td>
</tr>
<tr>
<td>Analytical Chem</td>
<td>CHEM 2114</td>
<td>118</td>
</tr>
<tr>
<td>Analytical Chem lab</td>
<td>CHEM 2124</td>
<td>94</td>
</tr>
<tr>
<td>Survey of Organic Chemistry</td>
<td>CHEM 2514</td>
<td>82</td>
</tr>
<tr>
<td>Organic chem</td>
<td>CHEM 2535</td>
<td>1068</td>
</tr>
<tr>
<td>Organic chem 2</td>
<td>CHEM 2536</td>
<td>0</td>
</tr>
<tr>
<td>Organic lab</td>
<td>CHEM 2545</td>
<td>1050</td>
</tr>
<tr>
<td>Organic lab 2</td>
<td>CHEM 2546</td>
<td>869</td>
</tr>
<tr>
<td>Pchem</td>
<td>CHEM 3615</td>
<td>240</td>
</tr>
<tr>
<td>Pchem lab</td>
<td>CHEM 3625</td>
<td>27</td>
</tr>
<tr>
<td>Pchem for Life Sciences</td>
<td>CHEM 4615</td>
<td>242</td>
</tr>
<tr>
<td>Pchem for Life Sciences 2</td>
<td>CHEM 4616</td>
<td>169</td>
</tr>
</tbody>
</table>

**Total "Service Course" enrollments**

<table>
<thead>
<tr>
<th></th>
<th>Fall 2011</th>
<th>Spring 2012</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total</td>
<td>8663</td>
<td>6172</td>
</tr>
</tbody>
</table>

### Highlights from Academic Year 2011-2012

#### Faculty Activities and Achievements

- **Prof. Daniel Crawford** received the 2012 Jimmy Viers Teaching Award, which was established by one of our alumni, E. Gary Cook, to recognize outstanding teaching in the Department of Chemistry. Prof. Crawford is honored for his exemplary efforts in general chemistry (majors section), and has the distinction of being the first two-time recipient of this award.

- **Prof. Preston Durrill**, Adjunct Prof. of Chemical Engineering and an Instructor in Chemistry, received the 2012 Sporn Award for Excellence in Engineering Education for the second time (he was also a 2006 Sporn recipient). VT’s Student Engineers’ Council selects one faculty member out of the more than 300 in the college to receive this honor. "Preston is the epitome of what an educator should be. He is a gifted teacher who has a remarkable passion for his students. We are truly fortunate to have him at Virginia Tech," said John Walz, Professor and Department Head of Chemical Engineering.

- **Prof. Gary L. Long** was one of two recipients of the University's 2011-2012 Scholarship of Teaching and Learning Award, which recognizes faculty members who have dedicated themselves to advancing higher education teaching and learning. Long remains committed to developing new technology and new ideas that better link the lab experience to learning gains in the chemistry classroom.

- **Prof. Timothy E. Long** was named Associated Dean for Strategic Initiatives, beginning January 2011, which involves renovation coordination and oversight, IGEP coordination, science-art initiative, ISC course and curriculum development and promotion, research team development, CARS/CAGS and Associate Dean Network.
✓ **Prof. Gary Long** will begin teaching in the Integrated Science Curriculum of the College of Science in 2011 - 2012. His work began in Summer 2011 with the design and development of the laboratories for the second year ISC students. He also serves as a lecturer in the ISC program for the chemistry component of the second year experience. **Prof. Tim Long** also taught in the ISC program in 2010 – 2011, and will continue in this capacity during the next academic year.

Grants in Teaching and Learning

✓ **Prof. Gary L. Long**, together with four colleagues in allied units (Jill C. Sible and Deborah S. Wilson of COS, Bevlee A. Watford of COE, and Kathryne D. McConnell of OAA), received a grant totaling $1.56 million to continue the Student Transition Engineering Program (STEP) at Virginia Tech. STEP aims to increase the number and diversity of STEM (science, technology, engineering, and math) graduates through retention strategies emphasizing academic success and engagement with the scientific process and community.

Student Activities and Achievements

✓ **Martha V. Blakely**, a senior with a near-perfect GPA who graduated in May 2012 with a double major in Chem/Biochem, was named the 2012 College of Science Outstanding Senior. This award goes to a graduating senior who demonstrates outstanding performance in academic achievement, extracurricular activities, and contributions of service to the university and community. She also received an academic excellence award from the chemistry department, and the James Lewis Howe Award—presented annually to an outstanding VT student in the Virginia Blue Ridge Section of the American Chemical Society. In Fall 2012, Ms. Blakely will become a PhD candidate at the University of Pittsburgh in their Orthopedics and Tissue Engineering Program. Martha also was the recipient of a $5,000 Thacker Scholarship from the ACC for her graduate studies this fall. The award honors outstanding student-athletes who have performed with distinction in both the classroom and on the playing field, while demonstrating exemplary conduct in the community. Martha was also selected to the ACC All-Academic Women’s Tennis team for the third consecutive year.

Other notable graduating seniors who won chemistry department academic excellence awards (with their future plans in parentheses) include:

✓ Andrea Carlini (UC San Diego, PhD), Ben Cherniawski (U Mass Amherst, PhD), Eliot Edling (VT, PhD), Kevin Hammond (LMU-DCOM, DO), Micah Howard (nursing school), Lindsay Johnson (Minnesota, PhD), Lindsay Maxwell (Vanderbilt, PhD), Levi May (VT, PhD), and Rachele Piedmonte (VT, PhD)

✓ Kerry DeMella won both the McGrath and Wightman/MII awards and will be joining Americorps in Florida. Levi May also won the ACS Division of Inorganic Chemistry Award.

✓ The Ogliaruso scholarship was awarded to Ms. Olivia Renaldo, who is now a rising sophomore.
The Department of Chemistry awarded a number of merit-based scholarships this year. These mostly go to rising senior chemistry majors based on GPA, with BS favored over BA because the former is more rigorous and difficult.

<table>
<thead>
<tr>
<th>Student</th>
<th>Scholarship Name</th>
<th>Semester/Amount</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atienza, Johnver</td>
<td>Chemistry Friends</td>
<td>Spring 2012 scholarship ($1000)</td>
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<td>Bernier, Chad</td>
<td>Chemistry Friends</td>
<td>Spring 2012 scholarship ($1000)</td>
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<tr>
<td>Bickel, Lyndsey</td>
<td>Chemistry Friends</td>
<td>Spring 2012 scholarship ($1000)</td>
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<td>Carlini, Andrea</td>
<td>Hopper-Harvie</td>
<td>Fall 2011 scholarship ($1000)</td>
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<tr>
<td>Cherniawski, Ben</td>
<td>Chemistry Friends</td>
<td>Fall 2011 scholarship ($1000)</td>
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<td>Davis, Rachel</td>
<td>Kinser &amp; Johnson</td>
<td>Fall 2011 scholarship ($1000)</td>
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<td>DeMella, Kerry</td>
<td>Kinser &amp; Johnson</td>
<td>Fall 2011 scholarship ($1000)</td>
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<tr>
<td>Diefenderfer, Liesi</td>
<td>Chemistry Friends</td>
<td>Fall 2011 scholarship ($1000)</td>
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<td>Edling, H. Elliot</td>
<td>Chemistry Friends</td>
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<td>Lee, Michael</td>
<td>Ellett</td>
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<td>Magruder, Kate</td>
<td>May</td>
<td>Fall 2011 scholarship ($1000)</td>
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<td>Maxwell, Lindsay</td>
<td>Walker</td>
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<td>May, Levi</td>
<td>Bilisoly</td>
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<td>Tydings, Christopher</td>
<td>Bilisoly</td>
<td>Spring 2012 scholarship ($1000)</td>
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</tbody>
</table>

Summer research scholarships ($2250) were awarded to (faculty mentors in parentheses): Brent Bostwick (Gandour), Kevin Hannon (Crawford), Diane Holden (Carlier), Sean Huynh (Brewer), Arianna Seabrooks-Matthews (Kingston), Dennis Shim (Yee) and Christopher Tydings (J. Morris). These competitive scholarships fund the students to take undergraduate research during the summer.

**General Chemistry 2011-2012**

The Department of Chemistry is committed to the highest level of undergraduate education that it can deliver and applies that commitment to the thousands of students who take our “service” courses (i.e., non-majors), as well as our own chemistry majors. In fact, our General Chemistry Program continues to offer the largest service course program at Virginia Tech.

- During the Fall 2011 semester, approximately 3200 students (predominantly freshmen) were enrolled in the first semester General Chemistry class, CHEM 1035. Another 350 students were enrolled in CHEM 1035 during the 2012 Spring semester, while 1400 students were enrolled in the second semester class, CHEM 1036. A search was conducted in Summer 2011 for another full-time General Chemistry instructor. Since this search was unsuccessful, in addition to permanent faculty members, we used three temporary instructors in the Fall 2011 semester and one temporary instructor in the Spring 2012 semester to help with this student load. We still need another full-time, permanent General Chemistry instructor.
All General Chemistry students were assigned common on-line homework assignments, marking the first time that all General Chemistry students had the same assignments. With the addition of the on-line homework, all General Chemistry instructors now have the means of assigning and grading homework in their large classes. All instructors for General Chemistry also worked together to have very similar tests so that there would be more consistency between sections. The ultimate goal is for all sections of General Chemistry to have the same tests as we move to common-time tests in the evening and a common-time Final Exam. This will be implemented in Spring 2014.

In the Spring 2012 semester, the one CHEM 1035 section and seven CHEM 1036 sections had recitations associated with them, led by junior or senior undergraduates. In addition to the regular 150 minutes of lecture instruction each week, the students attended a small group (35 students/recitation) recitation each Thursday. There were a total of 52 weekly recitation sections taught by 26 undergraduates. Each week, the students worked in groups on a worksheet designed to aid them in problem solving, followed by a weekly quiz. The teaching experience is very rewarding for the undergraduate recitation instructors. Funding for these recitations was provided by the Department to the tune of $24K from the royalty fund.

All General Chemistry students had the opportunity to obtain free tutoring in the Chemistry Learning Center (CLC), open four days a week, and staffed with the Graduate Teaching Assistants who serve as General Chemistry lab instructors. In addition to finding help in the CLC, students could also attend evening help sessions offered by most General Chemistry instructors on a weekly basis.

With the addition of the new laboratory fee, General Chemistry lab students were able to use advanced instrumentation (currently, GC-MS and atomic absorption instruments) not available in most freshmen level courses at our peer institutions. The new lab exercises built around this instrumentation better reveal what real chemists do on the job and raise the level of student experience above that in similar lab courses at other universities.

The Chemistry Department worked to schedule General Chemistry classes for the First-Year Experience Program in the College of Agriculture and Life Sciences, the Biological and Life Sciences Community (BLSC), and the College of Engineering Hypatia and Galileo communities, ensuring that student community members were grouped together in chemistry lecture and lab.

Chemistry majors and selected biochemistry majors took their own General Chemistry courses, CHEM 1055/1056. Honors students who wished to take General Chemistry for Honors credit took CHEM 1055H/1056H.

In the Fall 2011 semester, 2280 students were enrolled in 95 sections of the first semester General Chemistry lab, CHEM 1045; another 900 students were enrolled in CHEM 1045 during the Spring 2012 semester (38 sections). To accommodate the number of students needing CHEM 1045 lab, 8 sections of this lab were taught on Tuesday and Thursday evenings during the Spring 2012 semester, the second year in a row that evening sections were needed. We hired another General Chemistry lab technician to run those evening sections.
• The number of students enrolled in the Spring 2012 semester of CHEM 1046, second semester lab, was 1248. All sections of CHEM 1045/1046 lab were taught by GTAs. For the first time, in Spring 2012, nine undergraduate chemistry majors joined graduate students as GTAs in CHEM 1046. The addition of undergraduate lab instructors was quite successful. A member of the Chemistry Department writes the laboratory manual used for this course.

LEARNING: GRADUATE PROGRAMS

Graduate Program Overview

Programs. The Chemistry Department offers PhD, thesis MS, and non-thesis MS degrees. While we do not admit students directly into our MS program, students may change their degree status from PhD to MS for several reasons including inadequate academic performance to achieve or maintain doctoral candidacy, changes in career plans, or personal circumstances. About half of the MS graduates continue to the doctorate.

Students in the doctoral program choose from five subfields of chemistry as shown in the accompanying table. The distribution can be attributed to significant strengths in polymer science, computational chemistry, and organic/medicinal chemistry.

<table>
<thead>
<tr>
<th>Area of Study</th>
<th>Number (May 2011)</th>
<th>Number (May 2012)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analytical</td>
<td>16</td>
<td>20</td>
</tr>
<tr>
<td>Inorganic</td>
<td>11</td>
<td>14</td>
</tr>
<tr>
<td>Organic</td>
<td>40</td>
<td>37</td>
</tr>
<tr>
<td>Physical</td>
<td>35</td>
<td>24</td>
</tr>
<tr>
<td>Polymer-Organic</td>
<td>38</td>
<td>41</td>
</tr>
<tr>
<td>Terminal Masters</td>
<td>7</td>
<td>8</td>
</tr>
</tbody>
</table>

*Includes students in computational chemistry and polymer physics and characterization.

In addition to our five “major” subfields, Chemistry enjoys a strong relationship with the interdisciplinary Macromolecular Science and Engineering (MACR) degree program. About 30 MACR students are advised directly by CHEM faculty members, and therefore CHEM students often work side-by-side with MACR students in our laboratories. The complementary training of the MACR students provides a resource to CHEM students, and *vice versa*.

Funding. Chemistry graduate programs often enjoy significant support from teaching assistantships because of the high service-teaching load in the undergraduate laboratories. As shown in the accompanying table, 56% of our students are supported on GTA funds, while 36% are supported on a combination of research grants, fellowships, and scholarships.
Graduate Admissions. The CHEM Graduate Program aims to enroll about 30 new students each year. The following table illustrates our status in meeting this objective.

<table>
<thead>
<tr>
<th>Class</th>
<th># of Applicants</th>
<th># Accepted</th>
<th># Enrolled</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fall 2012</td>
<td>215</td>
<td>87</td>
<td>33</td>
</tr>
<tr>
<td>Fall 2011</td>
<td>220</td>
<td>75</td>
<td>24</td>
</tr>
<tr>
<td>Fall 2010</td>
<td>219</td>
<td>72</td>
<td>34</td>
</tr>
<tr>
<td>Fall 2009</td>
<td>221</td>
<td>84</td>
<td>36</td>
</tr>
<tr>
<td>Fall 2008</td>
<td>215</td>
<td>48</td>
<td>37</td>
</tr>
<tr>
<td>Fall 2007</td>
<td>170</td>
<td>67</td>
<td>26</td>
</tr>
<tr>
<td>Fall 2006</td>
<td>150</td>
<td>49</td>
<td>26</td>
</tr>
</tbody>
</table>

For the Fall of 2012, of 215 total applications, 195 were sufficiently complete to warrant full consideration. Typically 40% of our applicants are US citizens, and the others are mostly Chinese or Indian, with perhaps as many as 10% of Middle-Easterners. Their “stats” are fairly stable from year to year as the accompanying table shows.

### Recruiting and Admissions Data

<table>
<thead>
<tr>
<th>Year</th>
<th>GPA</th>
<th>N(GPA)</th>
<th>GRE V</th>
<th>GRE Q</th>
<th>N(GRE)</th>
<th>GRE CHEM</th>
<th>N(CHEM)</th>
<th>TOEFL</th>
<th>%F</th>
</tr>
</thead>
<tbody>
<tr>
<td>2012</td>
<td>3.32</td>
<td>91</td>
<td>65/56</td>
<td>86/79</td>
<td>122/82</td>
<td>774 (77)</td>
<td>25</td>
<td>96</td>
<td>35</td>
</tr>
<tr>
<td>2011</td>
<td>3.38</td>
<td>68</td>
<td>60</td>
<td>80</td>
<td>185</td>
<td>776 (77)</td>
<td>35</td>
<td>96</td>
<td>37</td>
</tr>
<tr>
<td>2010</td>
<td>3.39</td>
<td>71</td>
<td>55</td>
<td>80</td>
<td>198</td>
<td>732 (66)</td>
<td>36</td>
<td>95</td>
<td>39</td>
</tr>
<tr>
<td>2009</td>
<td>3.39</td>
<td>56</td>
<td>55</td>
<td>85</td>
<td>201</td>
<td>761 (73)</td>
<td>42</td>
<td>95</td>
<td>37</td>
</tr>
<tr>
<td>2008</td>
<td>3.36</td>
<td>60</td>
<td>55</td>
<td>82</td>
<td>187</td>
<td>726 (65)</td>
<td>14</td>
<td>93</td>
<td>46</td>
</tr>
</tbody>
</table>

* Data for applicants to the doctoral degree program in CHEM.
* Entry Yr is the calendar year (Spring, Summer, and Fall) that students were applying to enter.
* Average GPA for domestic students only, based on the undergraduate degree.
* N(GPA) is the number of domestic applicants on which the GPA average is based.
* Average of self-reported GRE Verbal and Quantitative averages, converted to percentiles parentheses. For 2012, two numbers are reported to reflect scores on the old-format and new-format exams, respectively.
* N(GRE) is the number of applicants who self-reported GRE scores in their applications. For 2012, the two numbers are for applicants who reported old-format and new-format scores, respectively.
* N(CHEM) is the number of students who self-reported CHEM Subject Test GRE scores.
* The average TOEFL score for the "internet-based test" (iBT). 100 is the Department’s minimum, and in 2012 no exceptions were made to this requirement. No applicants reported scores in the out-dated computer-based test (cBT) or paper-based test (pBT) formats.
* The percentage of females applicants.
In March 2012, the Department held its annual recruitment weekend. By all accounts from visitors, faculty members, and “graduate ambassadors” (current graduate students who host visiting prospective students), the weekend was an enjoyable event. Each year we work to improve the event. With our faculty spread across campus, we instituted a “speed dating” event with several faculty at tables in the Hahn South atrium. The energy and excitement created during the event led to many compliments from both visitors and faculty members; our “family” approach to chemistry was well portrayed and well received. In addition faculty members and graduate students presented posters on the work of their respective research groups, and students were provided with tours of laboratories and the Virginia Tech campus. Of the students who attended, about half have committed to join Virginia Tech in the fall. The table below shows the undergraduate colleges and universities represented by the weekend attendees. This data shows that the department has expanded beyond a regional reputation and is attracting serious attention from students across the nation.

<table>
<thead>
<tr>
<th>Colleges and Universities Represented at the 2011 – 2012 Graduate Recruiting Weekend</th>
</tr>
</thead>
<tbody>
<tr>
<td>Allegheny College</td>
</tr>
<tr>
<td>Arizona State University Tempe</td>
</tr>
<tr>
<td>Bloomsburg University</td>
</tr>
<tr>
<td>Bucknell University</td>
</tr>
<tr>
<td>California Polytechnic State University</td>
</tr>
<tr>
<td>College of Ozarks</td>
</tr>
<tr>
<td>College of William &amp; Mary</td>
</tr>
<tr>
<td>Concord University</td>
</tr>
<tr>
<td>Delaware State University</td>
</tr>
<tr>
<td>East Tennessee State University</td>
</tr>
<tr>
<td>Ferris State University</td>
</tr>
<tr>
<td>Furman University</td>
</tr>
<tr>
<td>Ithaca College</td>
</tr>
<tr>
<td>Longwood University</td>
</tr>
<tr>
<td>Manchester College</td>
</tr>
<tr>
<td>Mary Baldwin College</td>
</tr>
<tr>
<td>Murray State University</td>
</tr>
<tr>
<td>North Carolina State University</td>
</tr>
</tbody>
</table>

**Outcomes.** The Chemistry Department awards about 15 doctoral degrees per year, and about half as many MS degrees (table below). As these numbers imply, 7 - 8 of our students leave the program each year without a degree. The data in the table shows a large increase in doctoral graduates, reflecting a “bumper crop” of 20 PhDs awarded just in the Spring 2012 term. Presently, we can only ascribe this number to ordinary fluctuations.
Our MS graduates either find jobs or elect to continue their educations in other fields, which have included law, medicine, public health, statistics, industrial engineering, business administration, secondary education, and the ministry. The following table shows that our PhD graduates are generally quite successful in finding situations in which they can continue their career development in teaching and/or research within chemistry or allied fields.

<table>
<thead>
<tr>
<th>Number of Persons</th>
<th>Employer</th>
<th>Position</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3M Corporation</td>
<td>Research Scientist</td>
</tr>
<tr>
<td>1</td>
<td>Alliant Techsystems</td>
<td>Research Scientist</td>
</tr>
<tr>
<td>2</td>
<td>Army Research Laboratories</td>
<td>Research Scientist, Postdoc</td>
</tr>
<tr>
<td>2</td>
<td>Celanese</td>
<td>Research Scientist</td>
</tr>
<tr>
<td>1</td>
<td>Cincinnati Children’s Hospital</td>
<td>NIH Postdoc</td>
</tr>
<tr>
<td>1</td>
<td>Coca-Cola</td>
<td>Research Scientist</td>
</tr>
<tr>
<td>1</td>
<td>Collagen Matrix</td>
<td>Customer Service Rep</td>
</tr>
<tr>
<td>1</td>
<td>Dow Chemical Company</td>
<td>Research Scientist</td>
</tr>
<tr>
<td>1</td>
<td>Edgewood Chemical Biological Center</td>
<td>Research Scientist</td>
</tr>
<tr>
<td>1</td>
<td>Harvard University</td>
<td>Postdoc</td>
</tr>
<tr>
<td>1</td>
<td>NASA Ames Research Center</td>
<td>Postdoc</td>
</tr>
<tr>
<td>1</td>
<td>National Institute of Standards and Technology</td>
<td>Research Scientist</td>
</tr>
<tr>
<td>1</td>
<td>National Institutes of Health</td>
<td>Postdoc</td>
</tr>
<tr>
<td>1</td>
<td>Pennsylvania State University</td>
<td>Postdoc</td>
</tr>
<tr>
<td>1</td>
<td>Radford University</td>
<td>Assistant Professor</td>
</tr>
<tr>
<td>1</td>
<td>Self-Employed</td>
<td>Homemaker and Mom</td>
</tr>
<tr>
<td>1</td>
<td>Sensors in Medicine and Biology</td>
<td>Research Scientist</td>
</tr>
<tr>
<td>1</td>
<td>Transylvania University</td>
<td>Assistant Professor</td>
</tr>
<tr>
<td>1</td>
<td>Unemployed</td>
<td>May 2012 graduate</td>
</tr>
<tr>
<td>1</td>
<td>United States Air Force Academy</td>
<td>Associate Professor</td>
</tr>
<tr>
<td>1</td>
<td>University British Columbia</td>
<td>Postdoc</td>
</tr>
<tr>
<td>1</td>
<td>University of California, Irvine</td>
<td>Postdoc</td>
</tr>
<tr>
<td>1</td>
<td>University of Melbourne</td>
<td>Postdoc</td>
</tr>
<tr>
<td>1</td>
<td>University of Southern Mississippi</td>
<td>Postdoc</td>
</tr>
<tr>
<td>1</td>
<td>University of Stuttgart</td>
<td>Postdoc</td>
</tr>
<tr>
<td>1</td>
<td>Wake Forest University</td>
<td>Postdoc</td>
</tr>
</tbody>
</table>

Work is still underway to establish rigorous Student Learning Objectives (SLOs) for the CHEM graduate programs by interfacing a new system of SLOs with our programmatic milestones and with the Annual Student Reviews. Recent activity in the Graduate Education Committee was directed toward simplification of the system so that collection of the necessary data could be more efficient.
Graduate Program Highlights

This year, the Department instituted a new Travel Grant program for graduate students using funds from an endowed scholarship program. The students helped staff recruiting activities at their respective conferences. The following students received $1000 grants to attend the American Chemical Society’s Spring 2012 National Meeting in San Diego:

✓ Sean Hemp (TE Long)
✓ Wenyu Zhang (WL Santos)
✓ Daiqiang Xu (KJ Edgar)
✓ Swapnil Sheth (H Marand)

The following students received $500 grants to attend the American Chemical Society’s 2011 Southeastern Regional Meeting in Richmond:

✓ Akiko Nakamura (JM Tanko)
✓ Jeremy Stegall (PA Deck)
✓ Zhiyang Zhang (LA Madsen)

Graduate Program Challenges

Diversity. Our commitment to diversity has demonstrated success in the area of gender equity. However the same commitment has not translated to strong numbers of minority applicants or enrolled students. Besides the large number of students self-identifying as Asian (45%), we have only one representative each for the Hispanic, Native American, and African-American race categories. Again, however the scarcity of underrepresented minorities in our student body reflects the applicant pool.

The Big Move. The rebuilding of Davidson Hall required about a third of our graduate students to move to remote locations including the CRC. Students need to travel to Central Campus frequently to attend classes and seminars, hold meetings and exams, fulfill GTA obligations, and use instrumentation needed in their research. Using a combination of transportation resources, including public transportation (Blacksburg Transit) a departmental van, and personal vehicles, students have responded to this situation with outstanding professionalism. Diminished service provided by Blacksburg Transit during the summer months is proving problematic for many of our students.

Annual Evaluations and SLOs. An annual evaluation system has been developed to meet the standards required by the University and the Graduate School. Implementation was not meeting expectations, so the Graduate Education Committee changed the timing of the report deadlines so that faculty would not be tasked at unusually stressful periods (such as the end of the semester). The most significant challenge to implementation is coordinating the system with another mandate to develop and implement measurable student learning objectives which can be logged into the university’s online tracking system (WEAVE). We have the data we need, however, to be on schedule with the requirements of the Office of Academic Assessment.

Graduate Student Achievement and Awards

✓ Ryan Fortenberry (nominated by TD Crawford), Jianbo Hou (LA Madsen), Joshua Kittle (AR Esker), and Travis White (KB Brewer) received the 2012 CHEM Graduate Research Awards. Among these three productive students alone are over twenty co-authorships on published or submitted research articles.
Hannah Mallalieu (nominated by KJ Brewer), Elise Naughton (PA Amateis), Neeraj Patwardhan (HW Gibson) and Jeremy Stegall (C Santos) received the 2012 CHEM Graduate Teaching Awards. These students distinguished themselves for consistent excellence as GTAs, for work far exceeding expectations, and for leadership among their peers.

A new award was instituted to recognize service and outreach (engagement) by graduate students. Amanda Hudson (nominated by AJ Morris) and Akiko Nakamura (JM Tanko) are the inaugural recipients of the awards (2012).

Sean Hemp, a graduate student in Tim Long’s group, was recognized by the ACS Polymer Division for "Excellence in Graduate Polymer Research." He presented an oral lecture on "Phosphonium-containing Polyelectrolytes for Nonviral Gene Delivery" at the Spring 2012 ACS meeting in San Diego, CA.

Daiqiang Xu, a graduate student co-advised by Dr. Kevin Edgar and Dr. Richard Turner, was recognized by the ACS Cellulose Division for "Excellence in Cellulose or Renewable Materials Research." He presented an oral lecture on the "Regioselective Synthesis of Cellulose Esters" at the Spring 2012 ACS meeting in San Diego, CA.

Amanda Wilmsmeyer, a 5th year graduate student advised by Dr. John Morris, was recently honored with a “Best Presentation Award” at the 2011 Chemical and Biological Defense Science and Technology Conference in Las Vegas, which showcased new and dynamic developments in basic and applied research within the chemical and biological defense landscape.

### Notable Events or Programs Related to Graduate Recruitment and/or Education

**On October 07, 2012**, the Department organized a faculty retreat. The subject matter of the discussion was the graduate program. During the retreat, the faculty made a number of suggestions for changes or adjustments to course requirements and other features of the graduate program. The Graduate Education Committee considered all of these suggestions and responded with a set of recommendations to the faculty in April 2012.

Profs. PA Deck, JM Tanko, and GT Yee developed CHEM 6904 Generating Research
Ideas in the Fall of 2011. This course is a prerequisite to the department’s Original Research Proposal course (CHEM 6914) and is intended to help students understand how scientists formulate and evaluate new ideas for research proposals. Dr. Tanko took the leadership role in this development, introducing a schedule of written assignments, oral presentations, and faculty-led discussions. The outcome of this course development was evident in the ensuing Spring 2012 CHEM 6914 course, because all of the students in CHEM 6914 had their “main idea” approved by their faculty evaluators – a first.

✓ Prof. Richard Gandour and Angie Miller organized the Department’s annual Graduate Recruiting Weekend, held in March 2012.
✓ Our longtime Graduate Coordinator, Angie Miller, retired on May 01, 2012. A luncheon was held to honor Mrs. Miller on May 04.
✓ Our new Graduate Coordinator, Joli Huynh, joined our department on May 15, 2012. Mrs. Huynh brings a wealth of knowledge and experience to our department from her prior service in the Graduate School and the Registrar’s Office.
✓ Prof. Daniel Crawford developed a publicly accessible, self-guided, on-line tutorial system for teaching electronic structure theory to graduate and advanced undergraduate students. The system uses C/C++ programming as its foundation, but does not assume that the student has any significant background in programming. Prof. Crawford opened the site to the public in 2011, and it is now used by approximately 5-10 other research groups in theoretical chemistry.
✓ Prof. Paul Deck maintained and upgraded a database-driven website to track graduate student progress, featuring a paperless document filing system for the Graduate Coordinator’s office.

DISCOVERY

The Department of Chemistry remains an exceptionally active department in terms of research, as exemplified by research awards, funded grants, and research expenditures. What follows is a sampling of the many honors, awards, and funded programs associated with members of the Department of Chemistry.

Faculty Awards and Honors for Research

✓ Prof. John R. Morris is the recipient of the 2012 John C. Schug Research Award. This award was established by E. Gary Cook (a VT alum) to recognize faculty members who demonstrate exceptional creativity and productivity in their research. Prof. Morris’ research interests are in the broadly defined area of surface science, with particular emphasis on gas adsorption and
scattering from model surfaces, and gas-surface reaction dynamics with applications in the environment and in catalysis. Prof. Morris is the first chemistry faculty member to win all three major departmental awards for teaching (2010), research (2012), and service (2009).

✓ **Prof. Timothy E. Long** received four national awards/honors in 2011: (1) The Mark Scholar Award from the ACS Polymer Division, which recognized excellence in basic or applied research and leadership in polymer science; (2) the Pressure Sensitive Tape Council (PSTC) 2011 Carl Dahlquist Award for his research relating to adhesive tape technology; (3) an ACS PMSE Division (Polymeric Materials: Science and Engineering) Cooperative Research Award for excellence in polymer research in collaboration with industry; and (4) Dr. Long was also named an ACS Division of Polymer Chemistry Fellow for excellence in polymers and to the profession.

✓ **Prof. Daniel Crawford** has been awarded the 2012 Alumni Award for Research Excellence. This premier university award recognizes his significant contributions to theoretical and computational chemistry with applications to health science. Crawford has developed a series of quantum mechanical models capable of high-accuracy simulations of the interaction of polarized light with chiral molecules, a class of compounds that includes most modern medicines ranging from chemical sedatives to anti-tumor agents. These new computational tools will shorten the development time of new chiral drugs by years or even decade.

✓ **Prof. Daniel Crawford** was invited to give the prestigious 2012 Robert Mulliken Lecture to the Center for Computational Chemistry at the University of Georgia in April. His talk was provocatively entitled “Through the Looking-Glass, and What the Quantum Chemist Found There.”

✓ **Prof. John Morris** was selected as a Kavli Fellow—one of 122 of the nation's brightest young scientists from industry, academia, and government have been selected to take part in the National Academy of Sciences' U.S. and Chinese-American Kavli Frontiers of Science Symposia (November 17-19, 2011).

✓ **Prof. Tijana A. Grove**, was invited to present an honorary Young Protein Scientist Talk at the 25th Anniversary Symposium of The Protein Society, Boston, MA. July 23-27, 2011.

✓ In March 2012, **Prof. David Kingston** formally established the cross-disciplinary Virginia Tech Center for Drug Discovery (VTCDD). The vision of the Center is “To bring together the strong Virginia Tech capabilities in organic synthesis, infectious disease biology, polymer science, veterinary medicine, biomedical engineering, and our growing biomedical research capabilities in a collaboration to discover and develop new drugs to treat infectious diseases, neurological diseases, and cancer, as well as new methods of delivering drugs for these diseases, so that the resulting new chemical entities and delivery systems will be licensed and moved to clinical trials by a pharmaceutical partner.”

✓ **Prof. David Kingston**’s article, “Modern Natural Products Drug Discovery and Its Relevance to Biodiversity Conservation” (J. Nat. Prod. 2011, 74, 496–511), was selected for inclusion in a special thematic issue of Science for Environment Policy. The same article was also the third most downloaded article from the Journal of Natural Products in the last 12 months since its publication.

✓ **Prof. S. Richard Turner** successfully led the Macromolecules and Interfaces Institute (MII) through Office for the Vice President for Research (OVPR) reorganization, enabling it to remain one of only two “university wide” institutes on campus. Prof. Turner also presented MII achievements to the VT Board of Visitors Research Committee in March 2012.

✓ **Prof. Karen J. Brewer**’s recent work with photodynamic anti-cancer drugs was featured on the inside cover of the 21 September 2011 issue of *Chemical Communications*. Brewer identified a
supramolecule that can be activated by light during therapeutic treatments, which once activated binds to DNA and inhibits further cell replication. This discovery is important for developing drugs for diseases such as cancer, which can be treated by impeding cell replication. This finding also has implications for reducing the toxic side effects of certain cancer drugs.

✓ A September 2011 publication by Prof. Daniel Crawford and his University of Tromsø (Norway) colleague, Prof. Kenneth Rudd, was designated as a “very important paper” by the journal ChemPhysChem. Crawford and Rudd developed the most advanced computer model to date of the scattering of polarized light from chiral molecules. A long-term goal of this research is to enable chemists to carry out their own simulations to study compounds ranging from small molecules to pharmaceuticals and viruses.

✓ Prof. John R. Morris and his former graduate student, Jessica Lu, investigated reactions of ozone with an organic surface (a vinyl-terminated self-assembled monolayer). Their work was featured in early November 2011 on the cover of the Journal of Physical Chemistry C. This fundamental study, conducted with collaborator Prof. Richard D. Gandour and members of the Morris research group, used a series of molecular beam scattering experiments to provide insights into the fate of ozone in the environment.

✓ As highlighted in the 19 June 2011 “News and Views” segment of Nature Materials, Prof. Louis A. Madsen’s group has uncovered new aspects of the flow and filtering of water or ions in polymer membranes. This fundamental study, conducted with collaborator Prof. Robert B. Moore, has implications for a number of industrial applications that involve molecular filtering, such as fuel cells, water desalination membranes, and even the production of artificial muscles for robots.

Notable New Research Funding in 2011 - 2012

✓ The Foundation for the National Institutes of Health awarded $450,655 to Prof. Paul R. Carlier, a leader in organic and medicinal chemistry and a member of the Vector-Borne Disease Research Group at VT, to develop an entirely new strategy to kill the mosquito that transmits the malaria parasite. Carlier will collaborate with Prof. Jeffrey Bloomquist at the University of Florida as part of a larger three-year, $1.4 million effort entitled “Voltage-Sensitive Potassium Channel as a New Target for Mosquitocides,” to develop a new class of insecticides that will interfere with the mosquito's nerve signal mechanisms, thus preventing it from flying—and therefore biting, which is how the disease is transmitted.

✓ Prof. Louis A. Madsen and Prof. Theresa M. Reineke (University of Minnesota) received a three-year NSF grant ($420,000) to explore the biodistribution of polymeric drug delivery systems that include an image-enhancement "beacon" to indicate the location of the delivered drugs in medical diagnostic tests such as MRI. Dr. Madsen and his co-workers will study targeting into simulated tissues and cells using magnetic resonance measurements, which will facilitate the polymer design and synthesis efforts of the Reineke group.

✓ Prof. James E. McGrath received an NSF Major Research Instrumentation Award (MRI) totaling $255,265 for the "Acquisition of a Dual Size Exclusion Chromatography-Asymmetric Flow Field Flow Fractionation Instrument." Profs. Judy S. Riffle and S. Richard Turner, Prof.
Kevin J. Edgar (WSFP), and Prof. Richey M. Davis (CHE) are co-PIs on the award. These faculty members are also affiliated with the Macromolecules and Interfaces Institute (MII). The instrument will allow measurement of absolute molecular weights, intrinsic viscosities, degrees of branching, aggregation characteristics, chemical stability, and biodegradation information for a vast collection of chemical compositions.

Prof. Judy S. Riffle received a grant from NSF ($381,000) to develop block copolymers that can form complexes with small-molecule or nanostructures ranging from metals to metal oxides, hydroxyapatite (bone), tooth enamel, and cationic drugs. The overall goal of the work is to find new materials that can engage in controlled binding with specific biomaterials or facilitate drug delivery.

Prof. John Morris received a $436,000 award from Edgewood Chemical and Biological Center for his work on “Surface Chemistry of CWAs for Decon Enabling Science: Mechanisms, Kinetics, and Product Analysis.”

Prof. Daniel Crawford was awarded a $422,000 research grant from NSF to develop quantum chemical models of chiral molecules and their interactions with polarized light. The ultimate goal is to help laboratory chemists determine which "hand" (right vs. left) of a chiral compound delivers the best properties in applications ranging from fragrances to pharmaceuticals.

Prof. Harry W. Gibson was awarded a grant from NSF ($420,000) to study macromolecules in which branch points, crosslinks, or repeat units are made from mechanical connections (rotaxanes or catenanes) instead of covalent bonds. Dr. Gibson and his co-workers will explore the unique physical properties of these supramolecular polymers, which have potential applications in biomedical materials, coatings, and composites.

Prof. David Kingston received a Biodiversity Group Award from the National Institutes of Health in the amount of $575,000 to study "Biodiversity Conservation and Drug Discovery in Madagascar." He also received a supplement from the International Cooperative Biodiversity Group (NIH) for $315,000, targeted for “Evaluation of the IHVR/NPDI Plant Extract Collection”

Prof. S. Richard Turner was awarded $390,000 from the National Science Foundation (Division of Materials Research) to investigate “Sterically Congested and Stiffened Alternating Copolymers: Synthesis, Solution, and Solid-State Properties” (June 1, 2012).

Prof. Sungool Wi received an award from the ACS Petroleum Research Fund (PRF), New Directions (ND) Program in the amount of $100,000 for work on “Dynamic and Morphological Characterization of Reverse Osmosis Membranes.”

Prof. Tim Long received four new awards during this reporting period, as follows: (1) $20,000 for support of the IUPAC World Polymer Congress from the National Science Foundation; (2) $17,000 from Astro Terra for work on “Self-Healing Inflatable Extraterrestes;” (3) $50,000 from Techulon, Inc., for “Phosphonium-based Nucleic Acid Delivery Vectors;” and (4) a unrestricted research award from IBM in the amount of $25,000 for work involving polyesters.

Prof. Karen Brewer received funding from the Department of Energy in the amount of $402,154 for work on “Photoinitiated Electron Collection in Mixed-Metal Supramolecular Complexes: Development of Photocatalysts for H₂ Production.”
Published Papers (peer-reviewed, 2011 – present): 194


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dihydroxy-4,4’-diamino-biphenyl (hab) and 2,2’-bis-(3,4-dicarboxyphenyl) hexafluoropropane
96. Xie, W.; Geise, G. M.; Freeman, B. D.; Lee, H.-S.; Byun, G.; McGrath, J. E., Polyamide interfacial
composite membranes prepared from m-phenylene diamine, trimesoyl chloride and a new
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D.; Kingston, D. G. I.; Shaw, C., An endogenous bile acid and dietary sucrose from skin secretions
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and synthesis of antiproliferative eupolauridine alkaloids of ambavia gerrardii from the
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73. Guo, R.; Sanders, D.; Smith, Z.; Freeman, B. D.; McGrath, J. E. In Thermally rearranged (tr) aromatic polymer membranes for gas separation, American Chemical Society: 2011; pp PMSE-4.

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The molecular basis of selectivity for anopheles gambiae mosquitoes, American Chemical Society: 2011; pp AGRO-68.


Patents (2011-present):

During the reporting period, twelve patent disclosures were filed, seven of which had chemistry faculty as lead PI. Twenty-two patent applications were filed. Patents issued are summarized below:

3. Chlorine Resistant Desalination Membranes Based on Directly Sulfonated Poly(arylene ether sulfone) Copolymers, James E. McGrath (PI), et al., patent no. 8,028,842, issued 10/4/2011
4. Insecticidal Carbamates Exhibiting Species-Selective Inhibition of Acetylcholinesterase, Paul R. Carlier (PI), et al., patent no. 8,129,428, issued 3/6/2012.

Invited Lectures and Seminar Presentations (CY 2011-12): ~200

Among the approximately 200 invited lectures and seminar/meeting talks that Chemistry Department faculty delivered during the 2011-12 academic year, the following are highlighted:

Prof. Paul Carlier: Invited Lecture: “Designing Human-Safe Insecticides Against the Malaria Mosquito” Department of Chemistry, Winthrop University, November 17, 2011.


Prof. Alan Esker: "Polysaccharide-based Polyelectrolyte Adsorption onto Model Cellulose Surfaces," Max-Planck Institut fuer Kolloid und Grezflaechen Forschung, Golm, Germany, February 24, 2011; "Probing Polysaccharide and Enzyme Interactions with Cellulose," Biopolymers Program, Department of Chemical and Biological Engineering, Chalmers University of Technology, Gothenburg, Sweden, February 11, 2011.

Prof. Felicia Etzkorn: Virginia Commonwealth University, Richmond, VA, “Pin1: WW Domain


Prof. Tim Long: Prof. Long presented many invited lectures, including talks at Henkel, 3M, Kraton Polymers, Solvay, the Lord Corporation, and Allergan. Of particular note was his Mark Scholar Award Lecture at the ACS Meeting in Denver, an invited lecture at IUPAC in Puerto Rico, and an invited lecture at the Gordon Research Conference on Polymers.


Prof. Webster Santos: Invited Lectures (selected) as follows: “Copper-catalyzed regioselective boration of α,β-unsaturated carbonyl compounds with unsymmetrical, preactivated diboron reagent,” CNRS, Laboratoire de Chimie de Coordination, Toulouse, France, July 12, 2011; “The old problem of targeting RNA: Are peptide boronic acids the solution?” Universidad de Alcala de Henares, Madrid, Spain, July 18, 2011; “Multivalent branched peptide boronic acids inhibit RNA-protein interactions,” University of Nottingham, Nottingham, United Kingdom, July 20, 2011; “Copper-catalyzed regioselective boration of α,β-unsaturated carbonyl compounds with unsymmetrical, preactivated diboron reagent,” Durham University, Durham, United Kingdom, July 21, 2011; “Disrupting RNA-protein interactions with branched peptide boronic acids,” University of Cambridge, Cambridge, United Kingdom, July 27, 2011; “Copper-catalyzed borylation and inhibition of protein-RNA interactions,” Wayne State University,
Detroit, MI, October 5, 2011; “The chemical biology of targeting sphingosine kinase and HIV-1 RNAs,” University of Kansas, Medicinal Chemistry Department, Lawrence, Kansas, February 9, 2012.

Dr. Carla Slebodnick: Chaired a special session entitled "Would You Publish This?" designed to create dialog between service crystallographers on how to handle the many problems that can arise with non-routine structures, 2011 American Crystallographic Association Annual Meeting. New Orleans, LA, May 28-June 2.


**ENGAGEMENT**

**Faculty/Staff Service**

Faculty and staff members in the Department of Chemistry remain highly active in service to the Department, the College of Science, Virginia Tech, and the profession. In addition to the many typical service-related activities in which our faculty routinely engage (student advising, manuscript/grant reviews, editorships, external committee assignments, conference organization), a number of specific service-related achievements are highlighted below.

- **Profs. Tim Long, Bob Moore, and Richard Turner** planned and organized the World Polymer Congress for International Union Pure and Applied Chemistry, which took place on the Virginia Tech campus from June 24-29, 2012. With an estimated 1500 attendees and 340 invited lectures, it is the largest external international program ever brought to the university.

- **Prof. Daniel Crawford** was elected to a five-year term as the Secretary/Treasurer of the Physical Chemistry Division of the American Chemical Society (PHYS). The division has approximately 6,000 members worldwide. As part of his responsibilities, he redesigned the Division’s website: http://phys-acs.org/.

- **Prof. Daniel Crawford** hosted an international workshop for 20 attendees at Virginia Tech focused on quantum chemistry software development, sponsored by the National Science Foundation and the United Kingdom’s Engineering and Physical Sciences Research Council,
November 9-10, 2011.

Prof. Daniel Crawford served as president of the College of Science Faculty Association. He was charged by Dean Chang to revitalize the COSFA as an information conduit between his office and the faculty at large. This included his development of the “Dean’s Breakfast” series, the first of which was held in May 2011.

Prof. Paul A. Deck was selected as the 2011 recipient of the E. Ann Nalley Award for Volunteer Service to the Southeast Region of the ACS. The award, which was presented at the SERMACS 2011 Award Banquet on October 27 in Richmond, VA, recognizes the volunteer efforts of individuals who have contributed significantly to the goals and objectives of the American Chemical Society through their regional activities.

Ms. Melba Edwards received the 2012 Harold M. McNair Staff Service Award for the second time. Named in honor of Prof. Harold McNair, who served as head of the chemistry department from 1990-92, this award recognizes exemplary service by a member of our staff. Ms. Edwards serves in our bookkeeping office and oversees the department’s major accounts.

Prof. Hervé Marand received the 2012 Clifford Faculty Service Award. This award, named in honor of Prof. Alan F. Clifford who served as department chair from 1966-1981, recognizes outstanding service to the department. Prof. Marand has a long career of service, having served on both of the department’s elected committees (Executive and Personnel), numerous faculty search committees, ten years on the Graduate Honor Court, and has most recently participated in the Executive Development Institute—a university program to identify and mentor future leaders. Prof. Marand also serves as the Associate Chair of the Department of Chemistry.

Prof. Bob Moore served as Chair of the Polymer Division of the American Chemical Society during 2011.

K-12 Education and STEM Programs/Community and Student Engagement

Prof. Daniel Crawford continues to work with homeschool students on scientific education outside of the normal classroom environment. He will be organizing and hosting a science fair for homeschool students (up through high school age) in the New River Valley in 2012.

As part of his NSF CAREER grant, Prof. Lou Madsen continued developing activities to initiate scientific motivations in girls age 6-11. During summer 2011, his 2nd-year PhD student, Kacey McCreary, continued work on designing “exploration kits” for young girls. Kacey also worked refined an interactive (forum + resources) website to spread this program and interact with kids and parents (“www.playcreatediscover.vt.edu”). They participated in “Kids Tech University” on February 25, 2012 to test the program with ~ 400 kids ages 7-12 for an afternoon of learning.

Dr. Maggie Bobbitt Bump directed The Youth Experiencing Science (YES) summer program, which involved 27 rising 3rd – 7th graders in rural SW Virginia counties who worked in the laboratories at Virginia Tech. This is a highly valued leadership experience for the SURP undergraduates, which also provides a stimulating, enjoyable summer experience for the young scientists. All of the REU students participated in our YES workshop, during which they teamed with children from surrounding districts. This diverse group of young scientists came from public, private, and home schools. The children, mentored by the REU students, worked on four teams, Gascapades (density concepts), Got Green Milk (fluorescent labeling), Acid People (drug encapsulation), and Nylon Noodles (polymers). They presented their demonstrations to the public at Steppin’ Out, the local street fair in Downtown Blacksburg on August 5, 2011.

Prof. Karen Brewer continues to be actively engaged in outreach to the K-12 system. Each January or March she and colleagues host a series of visits for Blacksburg Middle School students to visit the department, see a demonstration and hear about the excitement of chemistry. She has been engaged in this activity for nine years now and finds it to be a good way to
continue our outreach to “young scientists.” She also prepares and distributes science activities the students take home in order to extend the reach beyond the classroom. Additionally, Brewer and students in CHEM 1056H have been engaged in developing new outreach activities for 8th grade students to assist teachers in instruction for the physical science SOLs. She has also been a Judge for the Blue Ridge Regional Science Fair for approximately 15 years serving to judge projects in many areas.

- **The Chemistry Club at Virginia Tech** received an Honorable Mention Award by the American Chemical Society for its activities during the 2010-11 academic year. Club events included chemical demonstrations and an open house during National Chemistry Week, a winery tour in the spring, and chemistry programs at area schools. The Chemistry Department proudly recognizes the efforts of Andrea Carlini (club president) and Dr. Maggie Bump (faculty advisor) for their commitment of time and energy in support of the chapter.

- **Prof. Patricia Amateis** presented Chemistry Shows to two groups of middle school students (80 students total) in Camp Imagination July 14 and 21, 2011. This is a summer day camp at Virginia Tech sponsored by the Center for the Enhancement of Engineering Diversity in the College of Engineering.

### The Department of Chemistry Advisory Council (DCAC)

![Department of Chemistry Advisory Council and Chemistry faculty, Fall 2011](image)

Active members of DCAC include Frank Akers (chair), Michael Borgerding, Bill Bryant, Josh Bryson, Elizabeth Calvey, William Coleman, Christopher Curfman, Deanne Emory, Erick Iezzi, Mitchel Koppelman, Joseph Layman, Wayne Ogden, Thomas Piccariello (chair-elect), Rob Shenton, Michael Smith, William Starnes, Joseph Thrasher, John Walz (Head, VT Chemical Engineering Department), and Dean Webster. Supporting members include Edwin Boudreaux, Andy Brink, Gary Cook, Joseph DeSimone, Jennifer Filbey, Michael Glasgow, Mary Gum, Philmore Robertson, Robert Schwerzel, John Yost, Scott Banks, Jerry Bass, Ronald Earp, John Fildes, and Mark Hammersla.

At the Fall 2011 meeting, DCAC initiated, with generous contributions by its membership, the James P. Wightman Chemistry Lecture Series Excellence Fund. Once endowed, this fund will support the visits of outstanding scholars and lecturers to the Virginia Tech campus to enhance the educational experience of students, faculty, and the community at large. DCAC members also contributed to the composition of a year-end e-mail sent to chemistry alums to solicit support for the department. Also, Tom Piccariello was selected to be the next chair of DCAC.
At the Spring 2012 DCAC meeting, in addition to planning, DCAC held separate meetings with graduate and undergraduate students, and provided feedback to the department about how current students viewed their experiences. DCAC also met with the chemistry faculty (excluding the chair, associate chair, and assistant chair) to provide confidential feedback to the department chair about the current state of the department. A Scholar site was set up to provide an electronic repository of DCAC-related business (minutes, etc).

**DIVERSITY**

**Some Notable Activities by Departmental Members to Promote Diversity**

In ways both “recognizable” and subtle, Chemistry faculty and staff remain committed to increasing diversity across the department and within the sciences. Professor Diego Troya continues to merit particular notice for his diversity efforts. He was elected Chair of the Hispanic Caucus of Faculty and Staff at Virginia Tech, continues to serve on the College of Science Diversity Committee, and is active on the University Committee of Virginia Tech’s Future Faculty program. This program brings to the Virginia Tech campus exceptional minority graduate students in all areas who are close to finishing. Once on campus, the visitors take part in workshops that prepare them for job interviews. He also nominated this year’s winner of the College of Science Diversity Award, Prof. Felicia Etzkorn.

Some additional diversity-promoting contributions by departmental members are listed below:

**Specific Diversity Activities, Awards and Honors**

- **Prof. Felicia Etzkorn** was awarded the College of Science Diversity Award for 2011-2012. She was honored for “her contributions to diversity in the College of Science and at other levels in the university, specifically for her efforts in the recruitment of diverse graduate students and faculty, for being an active and supportive mentor to underrepresented students and faculty in COS and elsewhere in the university, and for reaching out and making contributions that are beyond those that would benefit your own program.”

- **Prof. Amanda Morris** attended the Diversity Development Institute to earn a Diversity Ally Certificate. She also attended both the general Safe Zone training and Transgender 101 session to receive the status of an active SafeZone member and a SafeZone office location.

- **Prof. Tijana Z. Grove** attended both the general Safe Zone training and Transgender 101 session to receive the status of an active SafeZone member and a SafeZone office location.

- **Prof. Gary Long** received the “Excellence in Access and Inclusion Award,” from the University in 2011.

- In 2011, **Jeannine Eddleton** (soon to be Dr. Jeannine Eddleton) completed her 18th summer of teaching for ASPIRE/STEP (Student Transition into Engineering Program), one of the
many programs administrated by the Center for the Enhancement of Engineering Diversity under Dr. Bevlee Watford. She will continue to administer the lab program this coming summer for both engineering and COS students, which is expected to double in size.

✓ **Prof. John Morris** continued his work with the Multicultural Academics Opportunities Program (MAOP) by serving as the liaison between the Chemistry Department and the MAOP program. This effort involves circulating applications to interested chemistry faculty and encouraging them to work with a summer MAOP student.

✓ **Prof. Joe Merola** served on the Advisory Board for VT-NC AMP, the Virginia Tech/North Carolina Alliance for Minority Participation. He also led a workshop for minority students on how to write personal statements for graduate applications.

✓ **Prof. Judy Riffle** worked with focus regional universities to develop recruiting and research collaborations with schools that have high fractions of minority students: Funded programs have been established with St. Paul's College (HBCU), Lawrenceville, VA. This funding supported 3 summer undergraduates in 2011, and one Research Experiences for Teachers for a teacher from St. Paul's.

✓ **Prof. Patricia Amateis** presented a chemistry show to middle school students from Forest Park academy—primarily urban minority students from Roanoke who traveled to VT for the show.

✓ **Dr. Shamindri Arachchige** coordinated and hosted chemistry activities for the Virginia Tech Alliance for Minority Participation in August 2011.

**SAFETY**

Recent incidents such as the death of a lab worker at UCLA (2008) and an explosion and injury at Texas Tech (2010) have prompted many chemistry departments to take a fresh look at safety and chemical hygiene. In August 2011 the Chemistry Department Safety Committee began a thorough review of safety practices in our department. The committee is charged to gather information, recommend safety policies, disseminate information, and perform lab inspections. The safety committee chair meeting with the department chair and others in a weekly staff meeting further highlights safety.

The move of several groups to temporary space in RB26 at the Corporate Research Center led to new policies and personnel training. The chemistry stockroom now handles transport of chemicals to RB26 and ICTAS I. The departmental training coordinator, Patty Angus, arranges training from EHS personnel on six different topics each year. The breadth of creating a safe work environment in the Chemistry Department is non-trivial, encompassing many of the University-level EHS programs:

<table>
<thead>
<tr>
<th>Accident Investigation</th>
<th>First Aid</th>
<th>Radiation Safety</th>
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<tbody>
<tr>
<td>Biological Safety</td>
<td>Hazard Monitoring</td>
<td>Radioactive Material Safety</td>
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<td>Bloodborne Pathogens</td>
<td>Laser Safety</td>
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<td>Chemical Safety</td>
<td>Machine Shop Safety</td>
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<td>Electrical Safety</td>
<td>Nanomaterials</td>
<td>X-Ray Safety</td>
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<td>Fire and Life Safety</td>
<td>Personal Protective Equipment</td>
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**Highlights of the accomplishments of the Safety Committee include:**

- updates of door contact information and LCHO database
- installation of backup spill kits on each floor of Hahn South and in RB26
- peer inspections of all lab groups by student inspectors (Dec/Jan)
- incident reports transferred to online survey system to obtain yearly summary
- accident investigation of dropped 80-L liquid nitrogen dewar
FINANCIAL SUMMARY

Extramural Research Funding

As the following graphic shows, research funding for the Department of Chemistry fell dramatically in FY 2011—down 44% from the all-time high in FY2010. This decrease, and the concomitant decrease in research expenditures, is already impacting the department budget in the form of decreased overhead funding available (from ca. $40K/month in FY 10 to about $28 K/month at present, *vide infra*). With a spike in federal funding due to ARRA (stimulus funding) in FY09, part of this drop is certainly consistent with the national trend that many of federal research grants are expiring without being renewed. For comparison, the plot on the right illustrates funding provided by NSF’s Directorate for Mathematical and Physical Sciences: AST (astronomy), CHE (chemistry), DMR (materials), PHY (physics), OMA (multidisciplinary activities).

![Department of Chemistry Research Funding (FY 2006 – 2012)](image)

![NSF MPS Activity in Millions of Dollars FY 04 – FY12](image)

E&G, Overhead, and Discretionary Funding

Income for the Department of Chemistry is summarized below. Base funding remains frozen, and virtually every penny is used to fund basic operations such as salaries, services (communication network services, copying, undergraduate laboratories, etc.) Because of increased enrollments, summer school support has been steadily increasing. With the arrival of laboratory course fees for the general chemistry, enrollment support has started to decrease somewhat. The Department must however continue using overhead funds to support the education mission since caps on laboratory fees preempt us from recovering all laboratory expenses.
## Department Finances Summary

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<th>FY-06</th>
<th>FY-07</th>
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<td>2,912,746</td>
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<td>Summer School Total</td>
<td>129,200</td>
<td>134,917</td>
<td>155,436</td>
<td>196,520</td>
<td>220,653</td>
<td>238,247</td>
<td>273,733</td>
</tr>
<tr>
<td>Enrollment Support</td>
<td>106,068</td>
<td>150,963</td>
<td>371,750</td>
<td>580,214</td>
<td>712,273</td>
<td>933,169</td>
<td>884,019</td>
</tr>
<tr>
<td>Faculty Start Up</td>
<td>216,162</td>
<td>335,498</td>
<td>253,604</td>
<td>702,142</td>
<td>476,492</td>
<td>14,526</td>
<td>767,636</td>
</tr>
<tr>
<td>SCHEV Allocations</td>
<td>168,000</td>
<td>229,699</td>
<td>254,950</td>
<td>237,500</td>
<td>237,500</td>
<td>196,051</td>
<td>205,000</td>
</tr>
<tr>
<td>Overhead Return</td>
<td>333,702</td>
<td>288,241</td>
<td>239,746</td>
<td>392,905</td>
<td>471,524</td>
<td>452,690</td>
<td>340,910</td>
</tr>
<tr>
<td>Laboratory Course Fees</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td>257,000</td>
</tr>
<tr>
<td>Virginia Tech Foundation</td>
<td>4,670</td>
<td>5,680</td>
<td>8,050</td>
<td>2,550</td>
<td>6,050</td>
<td>14,000</td>
<td>8,400</td>
</tr>
<tr>
<td>Friends of Larry Taylor Account</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Virginia Tech Foundation</td>
<td>43,499</td>
<td>23,977</td>
<td>26,090</td>
<td>16,895</td>
<td>13,655</td>
<td>29,522</td>
<td>24,835</td>
</tr>
<tr>
<td>General Account</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Totals</td>
<td>5,491,026</td>
<td>6,294,992</td>
<td>6,459,976</td>
<td>7,351,772</td>
<td>7,290,400</td>
<td>7,099,826</td>
<td>8,062,297</td>
</tr>
</tbody>
</table>

### Undergraduate Laboratory Upgrades

Funding through a loan from the College of Science enabled a major upgrade to our undergraduate laboratories in FY11. The first phase of this upgrade included purchase of state of the art instrumentation (7 gas chromatographs/mass spectrometers, 6 atomic absorption spectrometers, 1 single quad LC-MS, and a 400 MHz NMR console). The magnitude of these purchases provided leverage, which helped the department negotiate a partnership with Agilent Technologies, a major instrument manufacturer, the benefits of which were detailed in last year’s report. As a result of this partnership, Agilent Technologies donated instrumentation valued at $250K including 1 Cary Eclipse fluorimeter, 1 Cary 100 UV-Vis spectrophotometer, 2 Value System 8453 UV-Vis spectrophotometers with diode arrays and Peltier cells, 1 971-FP flash purification system as well as 2 binary pumps, 1 variable wavelength detector, an autosampler and software for our single quad LC-MS.

In FY12, we renewed our partnership with Agilent Technologies and, through a second loan ($700K) from the College of Science, we were able to purchase a new 400 MHz NMR magnet with autosampler, 6 Cary 630 FT-IR spectrometers, 10 gas chromatographs with flame ionization detectors, 2 high performance liquid chromatographs with UV-Vis detectors, 1 Cary Eclipse fluorimeter, 4 Value System 8453 UV-Vis spectrophotometers with diode arrays, 2 atomic absorption spectrometers, and 12 Cary 60 UV-Vis spectrophotometers at discounts up to ca. 50% of list price. All our undergraduate laboratories
will share these instruments. The loan from the College of Sciences also allowed us to purchase a Rigaku Miniflex powder X-ray diffractometer, as well as a Mettler-Toledo Flash calorimeter for our upper undergraduate laboratories.

The Department will pay back these two large instrument loans to the College of Science using revenues generated by the undergraduate laboratory fees implemented in FY12 for the 1000 level labs, and extended in FY13 to the 2000 level labs. The table below provides detailed information about the revenues generated by these fees, 100% of which are used for the undergraduate laboratory activities. The information presented below also shows that to balance the budget of our general chemistry majors labs, the Department must complement the revenues received from lab fees by about $55K per year.

### Lab Fees, Revenues and Shortfalls:

<table>
<thead>
<tr>
<th>Course</th>
<th>Lab Fee per Student per Lab</th>
<th>Actual cost per Student per Lab</th>
<th># Students per Year</th>
<th>Lab Budget per Year</th>
<th>Annual Revenues from Lab Fees</th>
<th>Shortfall in Lab Funding per Year</th>
</tr>
</thead>
<tbody>
<tr>
<td>CHEM 1025/6 Intro to Chem.</td>
<td>$50.00</td>
<td>$50.00</td>
<td>132</td>
<td>$6,600</td>
<td>$6,600</td>
<td>$0.00</td>
</tr>
<tr>
<td>CHEM 1045/6 General Chem.</td>
<td>$55.00</td>
<td>$55.00</td>
<td>4257</td>
<td>$234,135</td>
<td>$234,135</td>
<td>$0.00</td>
</tr>
<tr>
<td>CHEM 1065/6 Freshman Maj.</td>
<td>$95.00</td>
<td>$113.42</td>
<td>189</td>
<td>$21,436</td>
<td>$17,955</td>
<td>$3,481</td>
</tr>
<tr>
<td>CHEM 2124 Analytical Life</td>
<td>$95.00</td>
<td>$102.74</td>
<td>197</td>
<td>$20,240</td>
<td>$18,715</td>
<td>$1,525</td>
</tr>
<tr>
<td>CHEM 2164 Analytical Maj.</td>
<td>$95.00</td>
<td>$176.10</td>
<td>63</td>
<td>$11,094</td>
<td>$5,985</td>
<td>$5,109</td>
</tr>
<tr>
<td>CHEM 2545/6 Organic Lab</td>
<td>$95.00</td>
<td>$95.00</td>
<td>2130</td>
<td>$202,350</td>
<td>$202,350</td>
<td>$0.00</td>
</tr>
<tr>
<td>CHEM 2555/6 SynTech Lab</td>
<td>$95.00</td>
<td>$683.39</td>
<td>61</td>
<td>$41,687</td>
<td>$5,795</td>
<td>$35,891</td>
</tr>
<tr>
<td><strong>Totals</strong></td>
<td></td>
<td></td>
<td><strong>7029</strong></td>
<td><strong>$537,542</strong></td>
<td><strong>$491,535</strong></td>
<td><strong>$46,007</strong></td>
</tr>
</tbody>
</table>

**Overhead Funds.** The Department receives 20.145% of overhead earned on sponsored research and uses the majority of these funds to support and enhance research in the department. These funds contribute towards the ca. 30 to 40% Department’s share of a new faculty member start-up package — and to maintain its current standard of excellence, the Department needs to hire two new faculty members per year. The following table summarizes overhead account expenditures for the past three years.
<table>
<thead>
<tr>
<th>Expenditures</th>
<th>2010</th>
<th>2011</th>
<th>2012</th>
</tr>
</thead>
<tbody>
<tr>
<td>Salaries</td>
<td>$160,783</td>
<td>$258,480</td>
<td>$132,721</td>
</tr>
<tr>
<td>GTA/GA</td>
<td>$67,226</td>
<td>$141,360</td>
<td>$26,741</td>
</tr>
<tr>
<td>T&amp;R Faculty</td>
<td>$24,492</td>
<td>$49,820</td>
<td>$30,484</td>
</tr>
<tr>
<td>T&amp;R Instructors</td>
<td>$1,327</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Post-Docs</td>
<td></td>
<td>$20,357</td>
<td>$34,177</td>
</tr>
<tr>
<td>Summer School Faculty</td>
<td>$52,056</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Staff</td>
<td></td>
<td>$10,950</td>
<td>$9,780</td>
</tr>
<tr>
<td>Wages</td>
<td></td>
<td>$10,378</td>
<td>$7,792</td>
</tr>
<tr>
<td>Fringes</td>
<td>$15,683</td>
<td>$25,615</td>
<td>$23,747</td>
</tr>
<tr>
<td>Administration</td>
<td>$86,952</td>
<td>$126,263</td>
<td>$182,615</td>
</tr>
<tr>
<td>Miscellaneous</td>
<td>$7,333</td>
<td>$3,034</td>
<td>$21,341</td>
</tr>
<tr>
<td>Building Maintenance</td>
<td>$9,374</td>
<td>$4,349</td>
<td>$6,113</td>
</tr>
<tr>
<td>Building Renovation</td>
<td>$3,306</td>
<td></td>
<td>$18,420</td>
</tr>
<tr>
<td>Chair’s Fund</td>
<td></td>
<td>$26,627</td>
<td>$2,635</td>
</tr>
<tr>
<td>Copying Cost</td>
<td>$2,614</td>
<td></td>
<td>$5,669</td>
</tr>
<tr>
<td>Delivery Service</td>
<td>$88</td>
<td>$114</td>
<td>$622</td>
</tr>
<tr>
<td>Faculty Recruiting</td>
<td>$21</td>
<td>$12,246</td>
<td>$221</td>
</tr>
<tr>
<td>Research Sponsor Default</td>
<td></td>
<td>$163</td>
<td>$45,206</td>
</tr>
<tr>
<td>Graduate</td>
<td>$43,851</td>
<td>$4,700</td>
<td>$71,123</td>
</tr>
<tr>
<td>Office Copier</td>
<td>$6,614</td>
<td>$633</td>
<td>$11,265</td>
</tr>
<tr>
<td>Alumni</td>
<td>$32</td>
<td></td>
<td>$0</td>
</tr>
<tr>
<td>Faculty Start-up</td>
<td>$19,409</td>
<td>$14,988</td>
<td>$126,981</td>
</tr>
<tr>
<td>Grad. Program</td>
<td>$34,100</td>
<td>$1,093</td>
<td>$1,600</td>
</tr>
<tr>
<td>Overhead-to-PI</td>
<td>$40,086</td>
<td>$48,259</td>
<td>$100,766</td>
</tr>
<tr>
<td>Service Centers</td>
<td>$1,574</td>
<td>$3,669</td>
<td>$11,837</td>
</tr>
<tr>
<td>Undergrad. Labs</td>
<td>$24,587</td>
<td>$43,643</td>
<td>$12,261</td>
</tr>
<tr>
<td>Undergrad. Prog.</td>
<td>$609</td>
<td>$862</td>
<td>$2,984</td>
</tr>
<tr>
<td>TOTALS</td>
<td>$368,131</td>
<td>$501,852</td>
<td>$571,765</td>
</tr>
</tbody>
</table>

The Department successfully recruited one new faculty member this year. Our startup package was clearly competitive, and we were able to achieve this without mortgaging the future, mainly because in addition to support from the College and Provost and use of the Equipment Trust Fund, we were able to assign our new faculty member some of the instrumentation left behind by Prof. T. Reineke, when she relocated to the University of Minnesota.

Nonetheless, various challenges are on the horizon. Generally, the Provost’s Office caps its contribution to start-up at $150K, with the balance split between Chemistry and the College of Science. Startup costs in chemistry (judged by our own experiences as well as information from our peers) are $600K and rising. The Chemistry Department lost a well-funded faculty member this year (Theresa Reineke). The federal
government has not been a reliable partner in research. Funding cuts, unstable politics in DC and expiration of American Recovery and Reinvestment Act (stimulus) funding has resulted in far fewer research awards to the department since November 2010. Several tenured faculty members are without, or are in danger of losing funding. It seems doubtful that the overhead budget will be able to support future activities at their current level. The time to plan is now if we are going to continue to hire chemistry faculty and sustain research.

The Department completed a philosophical discussion about the proper use of overhead funds. Two specific recommendations made by the Chair were voted upon by the Executive Committee and have been implemented during Spring 2012:

- Faculty members who lose research funding may be provided with bridge funding from the department overhead account for a period of one year upon successful petition to the Chair. Renewal of bridge funding beyond the first year will be considered on the basis of the faculty member’s record of submitted proposals and manuscripts published during the previous funding cycle.
- A small fraction of the overhead generated by the PIs will be returned to PIs.

**Stockroom Debt Repayment.** The Department paid its first annual installment of $26.7K on a loan contracted with the College of Science to relieve the Chemistry Stockroom debt that was incurred between 1999 and 2003. Pending an acceptable audit of billing procedures and practices in the Department, the College will contribute $55K of its own resources toward payment of this debt, which will be erased by the end of fiscal year 2016.

**Research Sponsor Defaults.** The Department finances were hit hard in 2011-2012 when two different research sponsors defaulted on their payment of contracted research expenditures. The total default (ca. $1.13M), was covered by the Office of Sponsored Programs (87%), the College of Sciences (6.7%) and the Department (6.7%) - our share, amounting to ca. $75K, will be paid over a 2-year period.

**Discretionary Funds.** Discretionary funds are used to support the broader mission of the department, specifically activities that cannot be supported by state funding. In a nutshell, these activities fund the "niceties" that lead to an intellectually stimulating and collegial environment for faculty, staff, and students. Discretionary funds are used to support or supplement the following activities:

- **Graduate Recruiting:** Successful research programs require a quality pool of graduate students. Despite our (historically) low stipend levels—both in comparison to other departments on campus and to our peer institutions nationally—we have found that our chances of attracting promising graduate students increase dramatically if we can get them to visit campus. Funds for graduate recruiting support prospective student visits to campus (travel, lodging), our "Graduate Recruiting Weekend" where we schedule visits en masse, and other activities aimed to increase the number and quality of our recruiting pool.
- **Undergraduate Activities:** In much the same way that we need high quality graduate students, the same holds true for undergraduates. Therefore, a portion of our discretionary funds is used to support undergraduate recruiting activities (for instance, booth rentals at local and national ACS meetings). Funds are also used to promote a friendly, inclusive atmosphere in the Chemistry Department where students can feel at home. For example, undergraduate students were invited to the recent chili cook–off and salsa competition.
- **Seminar Program:** A successful seminar program is the cornerstone of a successful Ph.D. program. Through its Highlands in Chemistry seminar series, the department brings scholars of national and international repute to present seminars and interact with faculty and students.
K-12 Outreach: Quoting from our mission statement: "Our outreach to the Commonwealth, the nation, and the world share our knowledge and expertise with scientists at all levels, form children in the early stages of their education to practicing professionals." Funds in this category are used to support faculty members who contribute to the community by either visiting local elementary, middle, and high schools or organizing on-site activities to share their knowledge of, and passion for, chemistry.

Faculty Recruiting and Retention: When recruiting new faculty, we feel it is important to pay their travel and lodging expenses, as well as arrange social activities so that we can get to know them better (and vice versa). Unfortunately, state reimbursement guidelines only allow us to go so far. Moreover, although the university funds new positions and a portion of research start-up costs, they do not provide any funds to cover faculty recruiting. This important activity is supported in part by discretionary funds. In rare cases, discretionary funds have also been used for faculty retention (equipment purchase, tuition payment, etc.).

Commencement Activities: A portion of our discretionary funds is used to support our yearly Spring Commencement Ceremony. This includes facility rental (we currently hold the Spring Commencement in the Lyric Theatre in downtown Blacksburg), cost of food/drinks for participants, and modest travel costs for our Commencement speaker.

Faculty, Staff, and Student Awards: In order to recognize the accomplishments of faculty, staff and students, and to keep morale high (especially important during times of disheartening budget reductions), the department uses its discretionary funds for monetary awards. Faculty awards are given to recognize excellence in teaching, research, and service. Staff awards are dedicated mainly to service. Student awards are given at both the graduate and undergraduate levels to recognize excellence in research, teaching, service, and other activities.

Social Activities for Undergraduate/Graduate Students/Staff/Faculty: With the goal of maintaining and improving collegiality and camaraderie in the department, we provide modest funds for activities and contests such as the best salsa competition, chili cook-off, etc., which we have found enhance departmental “good will” with minimal investment.

DCAC and Alumni Activities: Discretionary funds are used to defray the costs of the DCAC meetings (facility rental, meals, etc.), although it should be noted that DCAC members pay for their own travel and lodging expenses.

We have been extremely concerned about discretionary funds (VT Foundation dollars) available to the Department. As noted above, these funds are used to support the Highlands in Chemistry colloquium program, faculty recruiting, graduate and undergraduate student recruiting, K-12 outreach, the Department of Chemistry Advisory Council (DCAC) meetings, faculty & staff internal awards, scholarships, faculty retention, various social activities designed to maintain departmental morale, and the Department’s annual newsletter. The status and expenditures of discretionary funds are summarized below:

Between 2005 and 2010, the balance available to the Department had been decreasing by about $40K/year, which would mean the budget for these activities would have disappeared by ca. 2014. Beginning in FY11, we started, whenever possible, to charge a number of expenditures to our overhead fund rather than to the VTF funds. As can be seen on the next graph, this approach has led to a slowing down in the rate of decay of the discretionary fund balance. Note that the apparent ca. $190K increase in the balance of the Chemistry General Account shown in the above table is artificial as it reflects primarily some of the gifts in-kind received from Agilent Technologies.
### Status of the Chemistry VT Foundation Accounts:

#### Friends of Larry Taylor Endowed Account (886047) as of 05/30/12:

<table>
<thead>
<tr>
<th>Category</th>
<th>Amount</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carry-over from FY 2011:</td>
<td><strong>$ 62,323.79</strong></td>
</tr>
<tr>
<td>Gifts in FY 2012</td>
<td><strong>$ 8,400.00</strong></td>
</tr>
<tr>
<td>Unrealized+Realized Gains/Losses:</td>
<td>($ 1,944.52)</td>
</tr>
<tr>
<td>Income:</td>
<td><strong>$ 956.97</strong></td>
</tr>
<tr>
<td>Fees (Management/Administration/Assessment):</td>
<td>($ 1,213.91)</td>
</tr>
<tr>
<td>Endowment as of 05/30/12:</td>
<td><strong>$ 68,522.33</strong></td>
</tr>
</tbody>
</table>

#### Friends of Larry Taylor Income Account (873172) anticipated as of 06/30/12:

<table>
<thead>
<tr>
<th>Category</th>
<th>Amount</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carry-over from FY 2011:</td>
<td><strong>$ 11,798.40</strong></td>
</tr>
<tr>
<td>Income in FY 2012: (includes anticipated June income):</td>
<td><strong>$ 3,303.98</strong></td>
</tr>
<tr>
<td>Expenses in FY 2012:</td>
<td><strong>$ 0.00</strong></td>
</tr>
<tr>
<td>Income Account Balance (873172) anticipated as of 06/30/12:</td>
<td><strong>$ 15,102.38</strong></td>
</tr>
</tbody>
</table>

*Balance to be returned to principal at year end.

#### Chemistry General Account (881327) as of 05/30/12:

<table>
<thead>
<tr>
<th>Category</th>
<th>Amount</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carry-over from FY 2011:</td>
<td><strong>$ 105,291.79</strong></td>
</tr>
<tr>
<td>Gifts in FY 2012 as of 05/30/12:</td>
<td><strong>$ 24,835.00</strong></td>
</tr>
<tr>
<td>Gifts In-kind in FY 2012 as of 05/30/12:</td>
<td><strong>$ 221,277.71</strong></td>
</tr>
<tr>
<td>Expenses in FY 2012 as of 05/30/12:</td>
<td>($ 40,412.62)</td>
</tr>
<tr>
<td>Account Balance as of 05/30/12:</td>
<td><strong>$ 310,991.88</strong></td>
</tr>
</tbody>
</table>
The decline in monetary gifts received by the department observed between 2006 and 2010 appears to have stopped (see below), thanks an improving economy and possibly to a number of actions taken by the department:

- To better advertise and promote the Department, our web page underwent a major update. Links, and detailed instructions for online donations were added.
- The Chemistry Department newsletter (Elements) has been published regularly since Fall 2010 after a 2½-year hiatus. The intent is to continue publishing this newsletter near the end of each Fall and Spring semester (as long as funding permits). Note: In 2011 – 2012, only one issue was published (Spring 2012), but it was an expanded version relative to past issues. Moreover, our fund-raising appeal in Elements has become more aggressive.
- The Department of Chemistry Advisory Council was reinvigorated. Successful and productive meetings were held twice a year since November 2010. At the April meeting, DCAC revisited its mission, and began to develop a plan to assist the Department on various fronts.

While the apparent uptick in the balance observed 2010–12 is encouraging, it remains to be seen whether the success of these initiatives can be sustained or even grown to prevent the down-trend observed in the balance of our discretionary funds.
<table>
<thead>
<tr>
<th></th>
<th>Virginia Tech Foundation</th>
<th>Overhead Funds</th>
<th>E&amp;G Funds</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Expenditures</td>
<td>%</td>
<td>Expenditures</td>
</tr>
<tr>
<td>Alumni Newsletter and Chemistry Advisory Council Activities</td>
<td>$3,361</td>
<td>8.3</td>
<td>0</td>
</tr>
<tr>
<td>Faculty, Staff and Student Awards</td>
<td>$3,320</td>
<td>8.2</td>
<td>0</td>
</tr>
<tr>
<td>Graduate Recruiting</td>
<td>$15,588</td>
<td>38.5</td>
<td>$220</td>
</tr>
<tr>
<td>Departmental Activities for Graduate/Undergrad. Students/Staff/Faculty</td>
<td>$6,017</td>
<td>14.9</td>
<td>$966</td>
</tr>
<tr>
<td>Faculty Recruiting</td>
<td>$1,375</td>
<td>3.4</td>
<td>$221</td>
</tr>
<tr>
<td>Gift Assessment Fees paid to VTF</td>
<td>$1,738</td>
<td>4.3</td>
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</tr>
<tr>
<td>IUPAC 2012 World Polymer Congress Support</td>
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<td>12.4</td>
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<tr>
<td>Seminar Program</td>
<td>$1,662</td>
<td>4.1</td>
<td>$1,380</td>
</tr>
<tr>
<td>Undergraduate Recruiting</td>
<td>$611</td>
<td>1.5</td>
<td>$663</td>
</tr>
<tr>
<td>K-12 Outreach</td>
<td>$893</td>
<td>2.2</td>
<td>0</td>
</tr>
<tr>
<td>Commencement Activities</td>
<td>$130</td>
<td>0.3</td>
<td>$1,355</td>
</tr>
<tr>
<td>Miscellaneous</td>
<td>$750</td>
<td>1.9</td>
<td>0</td>
</tr>
<tr>
<td><strong>Totals</strong></td>
<td>$40,445</td>
<td>100</td>
<td>$4,805</td>
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</table>