# Department of Chemistry
## 2010-2011 Annual Report
### June 24, 2011

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<td>31</td>
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<td>- Patents Awarded (2010-present): 2*</td>
<td>40</td>
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Virginia Tech

Chemistry

Big Science

Solutions
EXECUTIVE SUMMARY

For the past year, despite a bad economy, budget cutbacks, and the impending renovation of Davidson Hall—Chemistry’s home for now approximately 80 years—the Department continues to excel at undergraduate and graduate learning, faculty discovery, diversity efforts, and engagement. In addition to a stellar group of faculty and staff spread across three buildings, the support of Prof. Hervé Marand (Associate Chair), Prof. Gordon Yee (Undergraduate Studies Director), Prof. Paul Deck (Graduate Program Director), Prof. Patricia Amateis (Director of General Chemistry) and Mr. Tom Bell (Assistant Department Chair) must be acknowledged. Their combined efforts have ensured that we exceed the needs of our students and faculty and continue to grow our reputation as a department of excellence. In addition, the efforts of Ms. Laurie Good in preparing this annual report are acknowledged and sincerely appreciated.

For the first time in three years, the Chemistry Department was in a position to hire new faculty members, and was successful in recruiting Drs. Amanda Morris and Tijana Grove. Amanda earned her B.S. from Penn State, Ph.D. from Johns Hopkins, and is wrapping up a postdoctoral position at Princeton. Her research will focus on the fundamental and practical aspects of solar energy conversion, and she will be teaching Electrochemistry in the fall. Tijana earned her undergraduate degree at the University of Belgrade, and her Ph.D. at Iowa State University. She is presently a posdoc at Yale University. Tijana’s research will deal with bioimaging and biosensors, and the design of nanoscale, ordered scaffolds for tissue engineering and drug delivery. She will be teaching Advanced Analytical Chemistry in the fall semester.

The Virginia Tech Department of Chemistry has a long history, a solid reputation and a bright future. Our courses provide the chemical foundation for all Virginia Tech science and engineering students and broaden their understanding about the structure and properties of matter. Our undergraduate and graduate degree programs prepare society’s future chemists and scientists. Our faculty’s research and scholarships generate and disseminate chemistry knowledge to the Commonwealth, the Nation and the world. Our outreach programs offer opportunities to share this knowledge with others, including practicing professionals, as well as primary and secondary school children. To achieve our mission, the Virginia Tech Department of Chemistry will continue to pursue multi-disciplinary research within and beyond the University, to find innovative ways to instruct students, to forge partnerships with industry and government, and to establish a reputation as one of the world’s highest ranking chemistry departments.

(Current mission statement of the Department of Chemistry at Virginia Tech)

Learning: Undergraduate

Our undergraduate program remains strong and is growing dramatically. In terms of the total number of undergraduate degrees awarded, the total number of B.S./B.A. graduates in Spring 2011 increased by almost half—from 60 during the year ending in 2010 to 89 this past May 2011.
Fall 2011 will mark the beginning of a major investment in education that will significantly improve the undergraduate laboratory experience for all our students. In the lab courses, our undergraduates will enjoy unprecedented hands-on access to major instrumentation early in their careers. For example, the general chemistry lab will use GC/MS to teach important concepts pertaining to isotopes and separations. We are the first in the nation to offer this level of hands-on experience in an introductory chemistry lab class. In the organic labs, our majors have always had access to NMRs in Syn-Tech lab (BS chemistry major lab). Starting this fall, our BA majors and non-majors will enjoy the same experience in the form of an undergraduate NMR lab, with a 400 MHz NMR as the centerpiece. Other improvements in the 2000, 3000, and 4000-level labs will be phased in over the next few years.

Learning: Graduate
The Chemistry Department’s graduate program offers up-to-date courses, amply-funded research opportunities mentored by internationally-recognized faculty members, and training for widely-varied career plans. The program serves a diverse student body of 150 students. We received approximately 220 applications and admitted 34 students in the Fall of 2010, while we graduated 15 students with PhD degrees and another 10 with MS degrees in the 2009-2010 academic year. Program highlights include the development and implementation of a web-based system for tracking applications and maintaining student records. In addition, initial implementation is underway for annual evaluation of all graduate students in accord with Graduate School policy, and for tabulating Student Learning Outcomes as prescribed by Southern Association of Colleges and Schools, the University’s main accrediting agency.

Discovery
The Chemistry faculty continues to build on a long and stellar tradition of discovery. Publications and presentations have increased and extramural research funding was over $12M in FY10. Despite a weak economy and uncertainties in federal funding, we appear to be on-track to match that amount in the next fiscal year. Departmental faculty members, staff, and even alumni were awarded a truly remarkable number of prestigious honors during this reporting period, which are detailed later in the report.

Engagement
In 2010-2011, faculty and staff in Chemistry engaged in notable leadership, service, and outreach for the profession, university, and wider community. Highlights include (1) The Macromolecules and Interfaces Institute (MII) Technical Conference and Review at Virginia Tech in Fall 2010, “Macromolecular Science and Engineering at Virginia Tech: Enabling a Healthy and Sustainable World,” (2) the announcement that Virginia Tech would be hosting IUPAC 2012 (International Union of Pure and Applied Chemistry) in May 2012 involving an estimated 1200 attendees, (3) the recent appointment of Prof. Timothy E. Long as Associate Dean for Strategic Initiatives in the College of Science, (4) the appointment of Prof. Robert Moore as the associate director of ICTAS, and (5) Prof. Gary Long serving this past year as president of the Virginia Tech Faculty Senate.

Diversity
The Department continues to pursue efforts that will enhance the recruitment and matriculation of undergraduate and graduate students from underrepresented groups. With respect the undergraduate program, of the recent 89 graduates in 2011, 40 were female (i.e., 45%). In terms of the graduate program, in addition to our 78 students from the U.S., ten other nations are represented in our student body, including significant numbers of Chinese (49) and Indian (11) students. The fraction of female applicants (ca. 40%) is close to the fraction of females currently enrolled (42%) suggesting that overall admission-and-retention in the Department is equitable with respect to gender. We expect our ability to recruit female students to improve dramatically with the recent hires of two female assistant professors. Additionally, an important achievement during this reporting year is the fact that Prof. Judy S. Riffle received the Virginia Tech College of Science Diversity Award for 2010.

Challenges for 2011-12 (and beyond)
Davidson Hall, home to Chemistry since the 1930s, is slated for a full renovation into a modern teaching-and-research building, leaving only the stone facade untouched. Funding to complete the design and for construction (Phase 1) will be available on July 1, 2011. Construction is expected to take place between January 2012 and January 2014 with substantial completion by year-end 2013. This impending renovation means that we must vacate the building and relocate staff, students, and faculty to other locations, as well as identify appropriate teaching rooms and research labs as needed. This has been an enormous challenge, but one that has had the full support of all involved. The challenge (and goal, as noted below) will be to continue to serve the thousands of majors and non-majors in our department, while at the same time ensuring that research activities are supported. (We remain hopeful that during this period, funding for Phase 2 will become available for renovation of the front portion of the building. Otherwise, the Department faces another disruptive set of moves).

Many of the research labs will be moving (this summer) to the Virginia Tech Corporate Research Center. At this moment, space in Research Building #26 is being prepared to house our labs at a cost to the University in excess of $2M—and we sincerely appreciate the assistance of the Provost’s office and College of Science in making this happen. We are also actively planning the relocation of faculty and administrative offices to other places on campus. The challenge for the department is that we will be fragmented over several locations for the next three years or so. And of course, we will need to evacuate Davidson Hall and be fully up and running for the fall semester!

Prof. Theresa Reineke, an associate professor here since 2008, has accepted an offer to join the faculty at the University of Minnesota, effectively immediately. Her work with drug delivery systems has brought her and her research group deserved recognition as demonstrated by impressive government and industrial funding, awards, invited lectures, etc. Her departure means that our polymer program will be challenged in terms of student advising, teaching, and funding levels. A request for a faculty position to fill this void has already been submitted to the College, and we are hopeful that this hiring effort could be coordinated with the Departments of Chemical Engineering and Materials Science and Engineering in the 2011 – 2012 academic year.
Goals for 2010 – 11: Status

In last year’s annual report, the following goals were outlined. Below is a status report, detailing what progress was made in the past year.

1. **Continue the excellent research activity for which the department is known. Work to expand those activities via strategic partnerships and alliances.**

By any measure (papers published, grants awarded, presentations, etc.) the Chemistry Department has indeed maintained excellence in research, as documented herein.

2. **Design and construction of Davidson Hall project will continue to be a large effort in 2010-2011. The final design has been approved by the Board of Visitors and is waiting funding by the state. A particular challenge to maintaining the excellence of the department in all of its dimensions will be the actual demolition and construction period of Davidson Hall. During that time, swing space in the Corporate Research Center will be used for research while the surge building will house departmental offices.**

The Davidson Hall project is on, the existing building will be vacated by the start of the Fall 2011 semester, and construction is scheduled to begin shortly thereafter.

3. **Recruit a faculty member who will add to our energy thrust and also add to the faculty diversity.**

“Soon-to-be Prof.” Amanda Morris was successfully recruited as an Energy & Environment cluster hire. In addition, Tijana Grove was recruited as a BioAnalytical Chemist.

4. **Expand the number of students engaged in undergraduate research.**

The number of undergraduates participating in undergraduate research has increased consistently over the past few years and was approximately 50 for each semester of the 2010-2011 academic year compared to an average of 23 and 36 in the preceding two years. To encourage even greater participation, research opportunities are discussed at Fall and Spring group advising sessions. Poster sessions and the end-of-semester undergraduate research symposium also give this activity greater visibility.

5. **Develop a more robust assessment program at all levels: faculty, staff, graduate student, and undergraduate students.**

The Chemistry department recognizes the need for more formal evaluation of teaching that goes beyond student perceptions of teaching (SPOT) scores. Exit interviews of graduating students and polls of the experiences of recent alums provide additional important perspectives. A final component that we are trying to implement is systematic peer
evaluations in which experienced teachers attend the lectures of colleagues and then provide both written and oral feedback. This process is mandatory for assistant and associate professors and our goal is two evaluations per faculty member per year. This procedure also provides an on-going written record of reviews for tenure and promotion dossiers.

6. Develop a new Department of Chemistry strategic plan ensuring that it aligns with the College of Science and University Plans.

The Executive Committee of the Department of Chemistry is now in the process developing a strategic plan. The Chemistry Department plans to be an important contributor both to the College and University strategic plans.

Goals for 2011-12

With the impending closing of Davidson Hall for total renovation, our primary goal for the upcoming year will be to ensure that our high standards of instruction, research, and erudition are minimally interrupted during the complex process of relocating staff, faculty, teaching labs, and experimental facilities to other locations on campus and at the CRC. Maintaining the collegiality and cohesiveness of the Department's faculty and staff during the renovation period when individuals will be scattered on and off campus is critical.

A major goal of the Executive Committee (EC) for the past semester was the development of a faculty-hiring plan that accurately reflected the Department of Chemistry’s current research ambitions and teaching needs. The success of the faculty searches in Spring 2011 has partially ameliorated the needs in analytical chemistry, and thus the EC focused the hiring plan in four areas: (1) macromolecular/polymer chemistry, (2) drug discovery, (3) computation/theory, and (4) energy and the environment. Each of these fits well with existing or emerging College of Science faculty clusters, and the department chair submitted a formal request to search in the first two areas beginning Fall 2011.

A second EC goal in spring 2011 was the construction of a departmental strategic plan that includes not only the faculty hiring priorities described above, but also to express our goals and the challenges we face in research, teaching, and outreach. Moreover, this plan needs to define how the Department will address the broader needs of society, as the field of chemistry evolves and national priorities shift. A fragile economy, coupled with the political environment in DC, has had (and will likely continue to have) a disruptive effect on research funding. The Department needs to chart a course that will not only enable it to weather these challenges, but allow it to improve in all areas of its mission with the long-term goal of becoming a top-ranked department nationally.

LEARNING: UNDERGRADUATE PROGRAMS

For the past year, Prof. Gordon Yee has served the Chemistry Department as Director
of Undergraduate Education. In that short period, he has become known as a tireless advocate for faculty and students (especially when it comes to awards and recognition) and organizing activities that have a positive effect on morale (the Department’s chili-cook-off, hikes, etc.). The department’s graduating BS/BA students have increased by nearly 50% in just one year, from 60 in 2010 to 89 in 2011. In terms of SPOT scores, the department's average SPOT score for all chemistry courses was 3.6; while the average SPOT score for all undergraduate chemistry course was 3.5.

As shown in the table below, our enrollment numbers have been comparable over the past three years, while the number of students declaring a Chemistry minor has increased by over 13% in just one year.

### Departmental Enrollment Trends

<table>
<thead>
<tr>
<th></th>
<th>Fall 02</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>
</tr>
</thead>
<tbody>
<tr>
<td>Primary CHEM majors</td>
<td>156</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>
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<tr>
<td>Secondary CHEM majors</td>
<td>34</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>
</tr>
<tr>
<td>TOTAL CHEM majors</td>
<td>190</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>
</tr>
<tr>
<td>CHEM minors</td>
<td>285</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>
</tr>
</tbody>
</table>
Chemistry Majors

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

*15 Honors-distinguished graduates among 60 in 2010 (25%)
*26 Honors-distinguished graduates among 89 in 2011 (28%)

General Chemistry 2010-2011

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 2010 semester, approximately 2900 students (predominantly freshmen) were enrolled in the first semester General Chemistry class, CHEM 1035. Another 300 students were enrolled in CHEM 1035 during the 2011 Spring semester, while 1400 students were enrolled in the second semester class, CHEM 1036. A full-time General Chemistry instructor, Dr. Shami Arachchige, joined the Chemistry Department in August 2010 to help with this student load.

- All General Chemistry students were assigned on-line homework with each of the many sections having one common on-line homework assignment each week. With the addition of the on-line homework, now all General Chemistry instructors have the means of assigning and grading homework in their large classes. Both semesters, 1-2 sections of CHEM 1035 also had recitations associated with them, led by junior or senior undergraduates. Problem-solving was the emphasis of the recitations.

- 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.

- The Chemistry Department worked to schedule General Chemistry classes for three Learning Communities, 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 course, CHEM 1055/1065; this section was also designated as the section for Honors students who wished to take General Chemistry for Honors credit.

- In the Fall 2010 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 2011 semester (39 sections). To accommodate the number of students needing CHEM 1045 lab, 8 sections of this lab were taught on Tuesday and Wednesday evenings during the Spring 2011 semester. This was the first time in several years that evening sections were needed. We were able to hire another General Chemistry lab technician to run those evening sections.

- The number of students enrolled in the Spring 2011 semester of CHEM 1046, second semester lab, was 1272. All sections of CHEM 1045/1046 lab were taught by GTAs. A member of the Chemistry Department writes the laboratory manual used for this course. Each year, 1-2 lab exercises are replaced by new lab exercises designed to interest and challenge our students.

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

**Service Course Enrollments**

As shown in the following table, the Department of Chemistry has a significant commitment to undergraduate non-majors on this campus. Although those two figures for Fall 2010 and Spring 2011 (totaling 15,089) do not represent individual students, they do indicate the importance of Chemistry’s role in instructing non-chemistry majors and ensuring that their own degree programs are enhanced by our instruction.
Fall 2010 and Spring 2011 Enrollments in our Service Courses (i.e., for non-majors)

<table>
<thead>
<tr>
<th>COURSE</th>
<th>Fall 2010</th>
<th>Spring 2011</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intro to Chem</td>
<td>CHEM 1015</td>
<td>358</td>
</tr>
<tr>
<td>Intro to Chem 2nd semester</td>
<td>CHEM 1016</td>
<td>340</td>
</tr>
<tr>
<td>Intro to Chem lab</td>
<td>CHEM 1025</td>
<td>78</td>
</tr>
<tr>
<td>Intro to Chem lab 2</td>
<td>CHEM 1026</td>
<td>57</td>
</tr>
<tr>
<td>Gen Chem</td>
<td>CHEM 1035</td>
<td>3137</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>2257</td>
</tr>
<tr>
<td>Gen Chem lab 2</td>
<td>CHEM 1046</td>
<td>1185</td>
</tr>
<tr>
<td>Analytical Chem</td>
<td>CHEM 2114</td>
<td>140</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>136</td>
</tr>
<tr>
<td>Organic chem</td>
<td>CHEM 2535</td>
<td>1074</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>1107</td>
</tr>
<tr>
<td>Organic lab 2</td>
<td>CHEM 2546</td>
<td>859</td>
</tr>
<tr>
<td>Pchem</td>
<td>CHEM 3615</td>
<td>188</td>
</tr>
<tr>
<td>Pchem lab</td>
<td>CHEM 3625</td>
<td>34</td>
</tr>
<tr>
<td>Pchem for Life Sciences</td>
<td>CHEM 4615</td>
<td>196</td>
</tr>
<tr>
<td>Pchem for Life Sciences 2</td>
<td>CHEM 4616</td>
<td>172</td>
</tr>
<tr>
<td><strong>Total &quot;Service Course&quot; enrollments</strong></td>
<td>8799</td>
<td>6290</td>
</tr>
</tbody>
</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.

Faculty and Departmental Teaching Awards

✓ Maggie B. Bump received the 2010 Jimmy Viers Teaching Award, which recognizes outstanding teaching by a departmental faculty member. Dr. Bump has developed recitations, guided learning activities, and interactive online homework to facilitate student engagement in 500-seat lecture sections of organic chemistry. She also advises the ACS Student Affiliates (SAACS), and students in her lecture courses earn credit for involvement in SAACS’s K-12 outreach. The award included a plaque and $1000.

✓ Dr. Michael A. Berg received the 2011 Viers Teaching Award. Dr. Berg's
contributions to the teaching mission of the department include large lecture sections of organic chemistry as well as the upper-division Drug Chemistry course. In characteristic fashion he ascribes much of his success in the classroom to the high aptitude and industry of his students. Additionally Dr. Berg serves as faculty advisor to dozens of undergraduates.

✓ Prof. Patricia Amateis was featured in the January 2011 issue of Virginia Tech Magazine. The article summarizes her long history of award-winning teaching and describes some of her classroom techniques, favorite demonstrations, and instructional philosophies.

✓ Prof. Daniel Crawford was selected as Virginia Tech “Scholar of the Week” for July 26-30, 2010.

✓ Prof. Gordon Yee received a Certificate of Teaching Excellence.

✓ Several members of the chemistry faculty were awarded the “Favorite Faculty Honor” by VT students.

Undergraduate Student Achievements and Awards

Max Hochenbury (who worked with Prof. Carlier) and Lilit Stepanyan (who worked with Prof. Brewer) each wrote and successfully defended honors theses in 2011. Lilit will be attending graduate school in chemistry at Stanford.

Leah Heist, a senior Chemistry major, was selected to receive the 2011 James Lewis Howe Award, presented annually to outstanding chemistry graduates of institutions located within the boundaries of the American Chemical Society’s Virginia Blue Ridge Local Section. Leah performed undergraduate research with Prof. Webster Santos and will attend graduate school in chemistry at the University of North Carolina.

Kasey Beernink, a senior CHEM BS major and a member of the Corps of Cadets, was a 2011 recipient of the “Advancing Women Award” from the VT Women’s Center. Nominated by her commanding officer, Kasey is recognized for her excellence and engagement in a Naval ROTC Unit and the Virginia Tech Corps of Cadets, and other notable extracurricular activities. Most notably, she was selected to serve as a nuclear submarine officer. The U.S. Navy opened submarine duty to women only last year, so she is one of a very few women in the entire nation to be selected for submarine duty. She successfully passed a rigorous battery of technical examinations and was hand-selected as a submariner by the Admiral directing the Naval Nuclear Propulsion Program. She will be the first Woman Submarine Warfare Officer to commission from Virginia Tech and her continued superior performance will undoubtedly pave the way for the others who come after her. In short, Kasey has “set the bar” for pioneering young women.

Jennifer Harvey was Named ESPN Academic All-American. Harvey, a senior CHEM BA major who also played on the women’s soccer team, earned a departmental academic award ($100) last year. Jennifer has earned an ACC postgraduate scholarship (The Weaver-James-Corrigan and Jim and Pat Thacker scholarships). Scholarships are awarded to selected student-athletes – three from each league.
institution – who intend to pursue a graduate degree following completion of their undergraduate requirements. Each recipient receives $5,000 to contribute to his or her graduate education. Those honored have performed with distinction in both the classroom and his/her respective sports, while demonstrating exemplary conduct in the community.

**Martha Blakely** was born in Bryn Mawr, PA. Martha majored in chemistry, economics and mathematics. She is the recipient of several awards ... the Skelton Award, given to the top Virginia Tech female scholar-athlete; she was named to the 2010 ESPN The Magazine Academic All-America Women’s At-Large Third Team; is one of 60 national winners of the Phi Kappa Phi Emerging Scholar Award; and was named to the 2009-10 All-ACC Academic Women’s tennis team. She also received the Frank Loria Award, given to only one Virginia Tech student-athlete annually who exemplifies outstanding leadership and scholarship.

The **Virginia Tech Chemistry Club** was awarded the ACS’s Green Chemistry Award and a Certificate of Achievement for their activities during the 2009-2010 academic year. From planning the annual chemistry shows and educational programs for elementary students to tie-dying lab coats and helping with the Davidson reunion in April, officers and members have been busy. The club did demonstrations at the Auburn and Gilbert Linkous elementary science fairs, and held chemistry workshops at Gilbert Linkous and Floyd elementary schools. Several events qualified the club for the Green Chemistry Award. Members planned a recycling activity that was done with 4th and 5th graders. Participants were able to separate different plastics based on their densities. Members also traveled to Kingsport, TN and toured Eastman Chemical, learning about industrial energy saving measures.

<Photo here>
ACS Green Chemistry Award: Virginia Tech Chem Club

**Grants in Teaching and Learning**

Working with Dean Jill Sible (COS), Gary Long was co-PI on an NSF STEP proposal entitled “Increasing STEM graduates in the physical and quantitative sciences at Virginia Tech.” The requested budget for this initiative was $1.9 M for five years, and the goal is to increase the number and diversity of STEM graduates in the COS through retention strategies that promote academic success and engagement with the scientific process and community. These strategies include. 1) a summer bridge program that provides academic enrichment and advising to prepare incoming freshman and transfer students for the rigors of their degree programs in science and 2) establishment of a freshman residential learning community for physical and quantitative science majors that complements the engineering and life science learning communities. As part of this program, the COS will enhance its first-year experience (FYE) program for transfer students to better serve the physical and quantitative science majors. (Note for the acronym-impaired: STEP = science, technology, engineering, and mathematics talent expansion program and STEM = science, technology, engineering, and mathematics.)
Notable Events or Programs Related to Undergraduate Education

- Shami Arachchige was hired as a permanent instructor for general chemistry, and a search is now in progress to fill a second position. Mike Berg and Vicki Long will move from temporary positions to the permanent instructor track, joining Maggie Bump and Jeannine Eddleton who were advanced in previous years. The stability of the instructor track, and the expectations for promotion in terms of scholarship and service will have a dramatic effect on the quality of the undergraduate program over the next few years. We acknowledge and appreciate the support received from the College of Science in support of these initiatives.

- The Chemistry Club (American Chemical Society Student Affiliates) organized a “Research Expo” that was held in the Hahn Hall Atrium in April. This was an undergraduate student poster session, which was held concurrent with a) the spring meeting of the Department of Chemistry Advisory Council (DCAC), and b) the Undergraduate Research Symposium. Our undergraduates did a superb job of highlighting the Department’s research activities for the DCAC meeting.

<Photo here>
Joe Calderone: Winner for “best poster” Research Expo 2011

- For nearly five years, Prof. Mike Berg has organized a tutor list every semester for organic chemistry. Tutors are students, undergraduates or graduates, who meet a certain set of criteria set up by the department and allowed to tutor-for-hire. Such activities are essential to the peer-led process of learning. Many students who are tutored, wish to tutor in the future and we believe this produces a positive atmosphere within the undergraduate mission of the department.

LEARNING: GRADUATE PROGRAMS

Graduate Program Update

Programs. The Chemistry Department offers doctoral, 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 academic performance, changes in career plans, or personal circumstances. About half of the MS graduates continue in the program and also earn doctorates, thus we graduate three or four “terminal” MS students per year. About a third of students who enter our doctoral program leave without a degree.

Students in the doctoral program choose from five “major” subfields of chemistry as shown in the accompanying table. The distribution can be attributed to significant strengths in the polymer science and organic/medicinal chemistry fields. It seems reasonable that the department would play to these strengths in its faculty hiring plans,
especially considering the pending departures and retirements anticipated in those areas.

<table>
<thead>
<tr>
<th>Area of Study</th>
<th>Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>Analytical</td>
<td>16</td>
</tr>
<tr>
<td>Inorganic</td>
<td>11</td>
</tr>
<tr>
<td>Organic</td>
<td>40</td>
</tr>
<tr>
<td>Physical&lt;sup&gt;a&lt;/sup&gt;</td>
<td>35</td>
</tr>
<tr>
<td>Polymer</td>
<td>38</td>
</tr>
<tr>
<td>Biochemistry&lt;sup&gt;b&lt;/sup&gt;</td>
<td>1</td>
</tr>
<tr>
<td>Terminal Masters</td>
<td>7</td>
</tr>
</tbody>
</table>

<sup>a</sup> Includes students studying computational chemistry and polymer physics and characterization.  
<sup>b</sup> Special category created for two biochemistry students who transferred from University of Cincinnati.

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 knowledge and 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. Thus, as shown in the accompanying table, 60% of our students are supported on GTA funds, while 33% are supported on a combination of sponsored programs, fellowships, and scholarships.

<table>
<thead>
<tr>
<th>Funding Stream (Total = $2.2 Million)</th>
<th>Number</th>
</tr>
</thead>
<tbody>
<tr>
<td>GTA</td>
<td>91</td>
</tr>
<tr>
<td>Research Grant</td>
<td>41</td>
</tr>
<tr>
<td>Fellowship or Full Scholarship</td>
<td>9</td>
</tr>
<tr>
<td>Self-supporting including students on Defending-Only Status</td>
<td>7</td>
</tr>
</tbody>
</table>

Graduate Admissions. The CHEM Graduate Program aims to enroll about 30 new students each year. Generally we only admit students intending to earn a doctoral degree. In approximate figures, of 220 total applications, 195 are sufficiently complete to warrant full consideration (see Table). Typically one-third of our applicants are Americans, and the others are mostly Chinese or Indian, with a “steady trickle” of Middle-Easterners (Turks, Egyptians, Iranians, Lebanese).

<table>
<thead>
<tr>
<th>Recruiting and Admissions Data&lt;sup&gt;a&lt;/sup&gt;</th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Year</td>
<td>GPA</td>
<td>N(GPA)</td>
<td>GRE V&lt;sup&gt;o&lt;/sup&gt;</td>
<td>GRE Q&lt;sup&gt;o&lt;/sup&gt;</td>
<td>N(GRE)</td>
<td>GRE</td>
</tr>
<tr>
<td></td>
<td>c</td>
<td>d</td>
<td>f</td>
<td>CHEM&lt;sup&gt;g&lt;/sup&gt;</td>
<td>h</td>
<td>i</td>
</tr>
<tr>
<td>----</td>
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<td>------------------</td>
<td>-------</td>
<td>-----</td>
</tr>
<tr>
<td>2011</td>
<td>3.38</td>
<td>68</td>
<td>497 (60)</td>
<td>734 (80)</td>
<td>185</td>
<td>776 (77)</td>
</tr>
<tr>
<td>2010</td>
<td>3.39</td>
<td>71</td>
<td>475 (55)</td>
<td>733 (80)</td>
<td>198</td>
<td>732 (66)</td>
</tr>
<tr>
<td>2009</td>
<td>3.39</td>
<td>56</td>
<td>473 (55)</td>
<td>757 (85)</td>
<td>201</td>
<td>761 (73)</td>
</tr>
<tr>
<td>2008</td>
<td>3.36</td>
<td>60</td>
<td>476 (55)</td>
<td>742 (82)</td>
<td>187</td>
<td>726 (65)</td>
</tr>
</tbody>
</table>

<sup>a</sup> Data for applicants to the *doctoral* degree program in CHEM.
<sup>b</sup> Entry Yr is the calendar year (Spring, Summer, and Fall) that students were applying to enter.
<sup>c</sup> Average GPA for domestic students only, based on the undergraduate degree.
<sup>d</sup> N(GPA) is the number of domestic applicants on which the GPA average is based.
<sup>e</sup> Average of self-reported GRE Verbal and Quantitative averages; percentiles in parentheses.
<sup>f</sup> N(GRE) is the number of applicants who self-reported GRE scores in their applications.
<sup>g</sup> CHEM is the average Subject Test GRE score. We do not require the Subject Test for admission.
<sup>h</sup> N(CHEM) is the number of students who self-reported CHEM Subject Test GRE scores.
<sup>i</sup> The average TOEFL score for the "internet-based test" (IBT). 100 is the Department's minimum.
<sup>j</sup> The percentage of females applicants.

In March 2011, the Department held its annual recruitment weekend, hosting 25 students from around the country. Poster sessions and meetings with faculty members introduced prospective students to our programs. Of the students who attended, about half have committed to join Virginia Tech in the fall.

**Outcomes.** The Chemistry Department awards about 15 doctoral degrees per year, and about half as many MS degrees (Table below). As these numbers imply, about one third of our students leave our program without a degree. Data recently collected in preparation for the submission of a proposal for an IGERT traininggrant show that only one of our degree recipients from 2008-2010 was unemployed. Our 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. Work is underway to establish rigorous Student Learning Objectives for the CHEM graduate programs by interfacing a new system of SLOs with our programmatic milestones and with the Annual Student Reviews. Implementation of this multi-purpose system is a complex challenge that we will tackle within the coming year.
### CHEM Graduate Degrees Awarded

<table>
<thead>
<tr>
<th>Degree</th>
<th>2010/11</th>
<th>2009/10</th>
<th>2008/09</th>
<th>2007/08</th>
<th>2006/07</th>
<th>2005/06</th>
</tr>
</thead>
<tbody>
<tr>
<td>MS</td>
<td>13*</td>
<td>10</td>
<td>5</td>
<td>10</td>
<td>4</td>
<td>5</td>
</tr>
<tr>
<td>PhD</td>
<td>12*</td>
<td>15</td>
<td>17</td>
<td>13</td>
<td>10</td>
<td>21</td>
</tr>
</tbody>
</table>

*Fall 2010 and Spring 2011

### Graduate Program Highlights.

- Full implementation of Graduate Applications and Student Progress databases. These are secure web-based tools for managing the large applicant pool efficiently, and for maintaining graduate student academic records, respectively. These systems were programmed by Michael Irwin, a Virginia Tech computer science major, who graduated in the Spring of 2011 and is now employed full-time by Virginia Tech Communications and Network Services as a Software Developer.
- Development of web-based tools for (a) accessing Materials Safety Data Sheets (MSDSs), (b) Reporting incidents and accidents, and (c) Requesting laboratory maintenance.
- Hire of a new student programmer, Titus Mawano, who is a rising junior computer science major. Mr. Mawano will help maintain, update, and upgrade the database systems designed and programmed by Mr. Irwin.

<Photo here>

Chemistry Department Commencement: Spring 2011

### 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, however. 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.
Rebuilding of Davidson Hall will move perhaps a third of our graduate students to remote locations including the CRC. Students will 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. The existing Blacksburg Transit service can provide some relief but will not be a complete solution.

#### Annual Evaluations and SLOs.
An annual evaluation system has been developed to meet the standards required by the University and the Graduate School, but has not yet been fully implemented. 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 are behind schedule on these implementations and need to assign them higher priority.
Graduate Student Recruitment

<table>
<thead>
<tr>
<th>Class</th>
<th>No. of Applicants</th>
<th>No. Accepted</th>
<th>No. Enrolled</th>
</tr>
</thead>
<tbody>
<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>

Average Standardized Test Scores for Accepted Graduate Students

<table>
<thead>
<tr>
<th>Entry</th>
<th>GPA</th>
<th>N(GPA)</th>
<th>Verbal</th>
<th>Quant</th>
<th>N(GRE)</th>
<th>CHEM</th>
<th>N(CHEM)</th>
<th>iBT</th>
<th>%F</th>
</tr>
</thead>
<tbody>
<tr>
<td>2011</td>
<td>3.38</td>
<td>68</td>
<td>497</td>
<td>734</td>
<td>185</td>
<td>776</td>
<td>35</td>
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<td>71</td>
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<td>198</td>
<td>732</td>
<td>36</td>
<td>95</td>
<td>39</td>
</tr>
<tr>
<td>2009</td>
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<td>56</td>
<td>473</td>
<td>757</td>
<td>201</td>
<td>761</td>
<td>42</td>
<td>95</td>
<td>37</td>
</tr>
<tr>
<td>2008</td>
<td>3.36</td>
<td>60</td>
<td>476</td>
<td>742</td>
<td>187</td>
<td>726</td>
<td>14</td>
<td>93</td>
<td>46</td>
</tr>
</tbody>
</table>

Notes:
- All data is for students requesting admission to the doctoral degree program. We admit so few students into a direct MS program that their data is not really meaningful.
- The Entry Year is the calendar year (Spring, Summer, and Fall) that students were applying to enter.
- GPA is the average for domestic students only, and is based on the undergraduate degree. These numbers are fairly consistent. The average includes students with GPAs less than 3.0 who are not even eligible to apply to our PhD program. We don't use MS GPAs in our average because those inflate the number artificially.
- N(GPA) is the number of students on which the GPA average is based. From this data you can see that domestic applications are trending slightly up (ca. 70) from 2008/2009 where they were around 60, possibly due to the recession of 2009.
- Verbal and Quant are the GRE averages, based on all applicants who self-reported GRE scores.
- N(GRE) is the number of applicants who self-reported GRE scores in their application. Generally we find that self-reported scores are accurate.
- CHEM is the average Subject Test GRE score. We don't required the Subject Test for entry, but some applicants take the exam and report the score.
- N(CHEM) is the number of students who self-reported CHEM Subject Test GRE scores.
- iBT is the average TOEFL "internet-based test" score. Nobody reports computer-based-test or paper-based-test scores any more.
- %F is the percentage of females in the applicant pool.

Graduate Student Achievement and Awards

- Zhenbin Niu, Giovanna Grandinetti, and Jing Wang received the 2011 CHEM Graduate Research Awards. Among these three productive students alone are over thirty co-authorships on published or submitted research articles.

<Photo here>

2011 Chemistry Department Graduate Research Award Recipients

- Kacey McCreary, David Hobart, and Furong Sun received the 2011 CHEM Graduate Teaching Awards. These students distinguished themselves for
consistent excellence as GTAs, for work far exceeding expectations, and for leadership among their peers.

<Photo here>

2100 Chemistry Department Graduate Teaching Award Recipients

- Furong Sun was awarded Best Oral Presentation in the Structural Biology, Biochemistry & Biophysics Section of the 2011 Virginia Academy of Sciences Annual Meeting, for her paper on phosphatidylinositol 3-phosphate recognition by the Phytophthora sojae effector Avh5. Furong is a fourth-year graduate student in Prof. Daniel Capelluto's research group.

- Yi Li, a graduate student in Prof. Richard Turner's research group, won the graduate category of the Fall 2010 OIRED/Phi Beta Delta International Experiences Speech Contest. In her speech "On a Journey Defining Myself," Julie reflected on the roles of language and networking, and on the value of persistence and openness.

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

- Prof. Lou Madsen developed CHEM 6664: TS: NMR Methods in Chemistry and Polymer Science, an all-new “special topics in physical chemistry” class. In addition to the 10 students who were graded for this class, 5-6 other students and faculty regularly attended his lectures and labs. This class was aimed at developing a more advanced understanding of how to choose and optimize NMR experiments for a range of characterizations. Knowledge of undergraduate physical chemistry, organic chemistry, and basic physics were required. Madsen incorporated an independent project to bolster ties between students’ research areas and NMR, and to enhance their writing and creative thinking skills for later PhD endeavors such as the Literature Review and Research Plan. In addition, he conducted 5 hands-on 3 hour laboratory sessions on state-of-the-art NMR instrumentation, covering theoretical and practical aspects of experiment choice and optimization, data collection, and data analysis and interpretation.

- Prof. John Morris organized the Department’s annual Graduate Recruiting Weekend, held in March 2011.

- Prof. Tim Long helped to organize the Graduate Recruiting Weekend (February and October) at the Fralin Institute, 2010.

DISCOVERY

The Department of Chemistry remains an exceptionally active department in terms of research, as exemplified by research awards, funded grants, and research expenditures. In fact, it is arguably one of the top research departments on campus. 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

✓ Prof. Karen J. Brewer, Professor Brenda Winkel (Biological Sciences) and Roger Dumoulin-White (Theralase Corporation) were named "Breakthrough Innovators" by Popular Mechanics for their work on light-activated compounds for the treatment of cancer. The magazine noted that "Two Virginia Tech scientists may have invented the future of cancer treatment - a way to eradicate tumors without the harmful side effects of chemotherapy, radiation or a surgeon's scalpel."

✓ Professor Harry C. Dorn's research program was featured on Virginia Tech's home page as a "Spotlight on Impact." The article describes the discovery and development, by Dr. Dorn and his team of collaborators, of methods to prepare tiny "buckyballs" of carbon that contain metal atoms. These nanomaterials show promising medical applications, including imaging and radiotracing. Dorn was also appointed as the Dr. A. C. Lilly, Jr. Faculty Fellow of Nanoscience. This endowed fellowship was established to provide support for an outstanding faculty member in the College of Science whose research is primarily in the nanoscience area. Dr. Dorn is known worldwide as a leader in carbonaceous nanomaterials including endohedral metallofullerenes and related species.

<Dorn Photo here>

✓ Prof. Timothy E. Long received the 2011 Mark Scholar Award from the American Chemical Society. This national award, named for legendary polymer scientist Herman Mark, recognizes Dr. Long's achievements in polymer synthesis and characterization for emerging technologies, including engineering thermoplastics, functional surfaces, fibers, and nanostructures. His interdisciplinary research approach interfaces developments in polymer science with biology and engineering.

✓ Prof. Judy S. Riffle received the university's 2011 Alumni Award for Excellence in Research. Riffle recognized for her significant contributions to the fundamental science of polymeric materials and for her interdisciplinary contributions to polymers in medicine. Her polymer research has led to the development of blood compatible materials, used in heart transplants and arterial grafts, and to highly oxygen-permeable extended-wear contact lenses. More recently, her research has focused on synthesis and assembly of core-shell nanostructures that carry therapeutic molecules or diagnostic agents in their cords. This approach allows for the independent molecular design of cores that will interact with the therapeutic/ imaging agents and coronas that interact with the physiological and cell environments.

✓ Professor Webster L. Santos was appointed the Blackwood Junior Faculty Fellow of Life Sciences. This fellowship was established to support and advance instruction, research and collaboration in the life sciences, with a complementary focus on the development of entrepreneurial opportunities. Dr. Santos's research focuses on the design of cell permeable RNA ligands as anti-HIV therapeutics and the development of sphingosine kinase inhibitors for the treatment of
hyperproliferative diseases such as cancer.

Webster Santos

✓ Prof. David Kingston’s article “Modern Natural Products Drug Discovery and Its Relevance to Biodiversity Conservation”, published in Marcy 2011, was one of the top ten most-accessed articles in the Journal of Natural Products in the last 12 months, and the third most-accessed article in March 2011.

✓ Prof. Judy S. Riffle was named a Fellow of the American Chemical Society Polymer Division. The award recognizes her many contributions to research and education in polymer sciences, as well as her long record of service to the Division.

✓ Professor Tim Long received the 2010 PMSE Cooperative Research Award (shared with Kraton Polymers).

Notable Research Awards

✓ Prof. James E. McGrath was one of ten winners of the Chief of Naval Research Challenge, a competition organized by the Office of Naval Research to identify research programs with the strongest potential to meet the current and future technological needs of the US Navy. Dr. McGrath and his co-workers in the Chemistry Department and the Macromolecules and Interfaces Institute (MII) will use the $100,000 award to investigate chlorine-resistant membranes for reverse and forward osmosis, nanofiltration, and waste water purification.

✓ Prof. Edward Valeev received a four-year NSF grant ($400,000) to work with collaborators at Stanford and Iowa State to develop sustainable software infrastructure for electronic structure theory. Their objective is to enhance the accuracy of the existing methods for describing weak intermolecular interactions and light-driven processes by creating sustainable software elements integrated into large community software packages.

✓ Prof. Louis A. Madsen received a three-year NSF grant ($324,000) to investigate dynamic ion-transport behavior in supramolecular materials with long-term applications in organic batteries and fuel cells. This work is part of an IUPAC-affiliated collaboration with Profs. Martin Moller (synthesis -- Aachen, Germany) and Dimitri Ivanov (structural characterization -- Mulhouse, France).

✓ Prof. Louis A. Madsen earned a $475,000 National Science Foundation (NSF) Faculty Early Career Development (CAREER) Award. Madsen's research focuses on improving advanced polymers for fuel cells and reverse-osmosis water purification by combining detailed analysis of these materials with theoretical understanding. CAREER awards are made to outstanding young faculty members who present career development plans that effectively integrate research and education, with an emphasis on combining the excitement of research with inspired teaching. Madsen’s project plan encompasses education
of promising university students and will build an outreach program specifically for girls in elementary school and their parents.

✓ Professor Webster L. Santos and collaborator David Rekosh (University of Virginia) received a five-year research grant from the National Institutes of Health in the amount $1.58 million to develop cell permeable, medium-sized molecules that target RNA structures essential for the HIV-1 life cycle. The research could lead to HIV/AIDS therapies.

✓ Professors Webster L. Santos, Hans Robinson (Physics), and Richey M. Davis (Chemical Engineering) received a three-year NSF grant ($500,000) to develop methods of assembling complex nanostructures. The project aims to demonstrate a new class of "patchy particles" having surfaces patterned with discrete interaction sites that attract or repel complementary sites on other particles. The long-term objective is to guide the self-assembly of complex structures with high precision and in high yield.

✓ Prof. Daniel Crawford received funding from the National Science Foundation in the amount of $2M, for “MRI-R2: Acquisition of a Heterogeneous Supercomputing Instrument for Transformative Interdisciplinary Research.” He will have access to the new machine, which is GPU-based and called “HokieSpeed”.

✓ Prof. John R. Morris has received a grant from NSF for molecular beam studies of surface chemical reactions. The $430,000, three-year award will help Dr. Morris and his co-workers further molecular level understanding of how common atmospheric pollutants react on surfaces of environmentally important organic materials, including surfactant-coated water droplets or aerosols, soot particles, and polymers.

✓ Prof. Karen Brewer received an award totaling $360,000 over two years from Phoenix International Energy, Inc. for her work on “A System for Light Driven Production of Hydrogen from Water.”

Published Papers (peer-reviewed, 2010 – present): 105


19. Fu, W.; Wang, X.; Azuremendi, H.; Zhang, J.; Dorn, H. C., 14n and 45sc Nmr Study of Trimetallic Nitride Cluster (M3n)6+ Dynamics inside a Icosahedral C80 Cage, Chemical Communications (Cambridge, United Kingdom) 2011, 47 (13), 3858-3860.


38. Niu, Z.; Huang, F.; Gibson, H. W., Supramolecular Aa-Bb-Type Linear Polymers with Relatively High Molecular Weights Via the Self-Assembly of Bis(M-Phenylene)-32-Crown-10 Cryptands and a Bisparaquat Derivative, Journal of the American Chemical Society 2011, 133 (9), 2836-2839.


81. McLendon, P. M.; Buckwalter, D. J.; Davis, E. M.; Reineke, T. M., Interaction of Poly(Glycoamidoamine) DNA Delivery Vehicles with Cell-Surface Glososaminoglycans Leads to Polyplex Internalization in a Manner Not Solely Dependent on Charge, Molecular Pharmaceutics 2010, 7 (5), 1757-1768.


90. Monceaux, C. J.; Carlier, P. R., Regioselective Synthesis of Aniline-Derived 1,3- and C1-Symmetric 1,4-Diols from Trans-1,4-Cyclohexadiene Dioxide, Organic Letters 2010, 12 (3), 620-623.


104. Sizovs, A.; McLendon, P. M.; Srinivasachari, S.; Reineke, T. M., Carbohydrate Polymers for Nonviral Nucleic Acid Delivery, Topics in Current Chemistry 2010, 296 (Nucleic Acid Transfection), 131-190.

105. Carlier, P. R.; Hsu, D. C.; Bryson, S. A., Self-Regeneration of Stereocenters (Srs) Via Stereolabile Axially Chiral Intermediates, Topics in Stereochemistry 2010, 26 (Stereochemical Aspects of Organolithium Compounds), 53-91.

Published Abstracts and Preprints (2010 – present): 101


51. Murphy, E. B.; Gao, R.; Inglefield, D.; Ramirez, S. M.; Long, T. E., Modification of Multi-Walled Carbon Nanotubes with Supramolecular Functionality for the Design of


63.  Hickory, B. S.; Deck, P. A., Mechanistic Investigation of the Simultaneous Oxidation and Coupling of 1,2,4-Tris(Pentafluorophenyl)Cyclopentadiene, Abstracts, Joint 66th Southwest and 62nd Southeast Regional Meeting of the American Chemical Society, New 2010, SESW-976.


73.  Smith, A.; Sizovs, A.; Xue, L.; Reineke, T. M., Glycopolycations Created Via Raft Polymerization Are Serum Stable and Effective Sirna Delivery Vehicles, PMSE Preprints 2011, No pp given.

74.  Allen, M. H.; Green, M. D.; Long, T. E., Tailoring Molecular Assembly of Imidazolium Copolymers and Nucleic Acids with a Synergy of Electrostatic and
Hydrogen Bonding Interactions, Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) **2011**, 52 (1), No pp given.

75. Bryson, J.; McLendon, P.; Reineke, T. M., _Luminescent and Mri-Active Polymers for Imaging DNA Delivery in Cells and Tissues_, Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) **2010**, 51 (1), 785.


82. McGrath, J. E.; Freeman, B. D., _Polymeric Membranes for Energy and the Environment_, Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) **2010**, 51 (1), 686-687.


84. Mittal, A.; Gibson, H. W.; Lee, M.; Choi, U. H.; Colby, R. H.; Salas-de la Cruz, D.; Winey, K. I., _Designing and Developing Imidazolium-Based Monomers for Ion- Conducting Polyelectrolytes_, Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) **2011**, 52 (1), No pp given.

86. Smith, A. E.; Sizovs, A.; Grandinetti, G.; Reineke, T. M., Diblock Glycopolymer Gene Delivery Vehicles Synthesized Via Raft Polymerization, Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) 2011, 52 (1), No pp given.


88. Zhang, M.; Long, T. E., Novel Sulfonated Segmented Block Copolyesters as Thermoplastic Elastomers in Biomedical Applications, Polymer Preprints (American Chemical Society, Division of Polymer Chemistry) 2011, 52 (1), No pp given.


Patents Awarded (2010-present): 2*


*Does not include others currently in the patent-pipeline—either as filed applications or patent disclosures.

Number of Invited Lectures and Seminar Presentations (CY 2010): ~200

Among the approximately 200 invited lectures and seminar/meeting talks that Chemistry Department Faculty delivered during the 2010 calendar year, the following are highlighted:


Prof. Daniel Crawford: “Recent Advances in Many-Electron Theories,” Raman Center for the Atomic, Molecular, and Optical Sciences, Kolkata, India, January 2010.


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 engage (student advising, manuscript/grant reviews, editorships, external committee assignments, conference organization), a number of specific service-related achievements are highlighted below.

 ✓ Prof. Joseph Merola stepped down as chair in August 2010, after six years of service to the Chemistry Department. During his tenure, Prof. Merola paid off an overhead and an E&G loan while hiring six new tenured or tenure-track faculty—nearly all of whom have been very successful in terms of funding such as CAREER awards and other prestigious awards such as Sloan fellowships. The Chemistry Department was named a University Exemplary Department during his tenure, and he was instrumental in the new design for the Davidson Hall renovations.

 ✓ Roberta Gilbert received the 2011 Harold M. McNair Staff Service Award. Ms. Gilbert was recognized for her outstanding service to the Chemistry Department as Business Manager, and especially for her contributions to maintaining the Department’s increasingly complex budget in view of University financial and auditing policies.

 ✓ Prof. Gary L. Long received the 2011 Alan F. Clifford Faculty Service Award in the Chemistry Department. The award recognizes a faculty member whose contributions exemplify the standards of selfless service demonstrated by Prof. Clifford during his career. Dr. Long’s distinguished record of service includes regional outreach through the Mobile Chemistry Laboratory, campus-wide pre-pharmacy student advising, and most recently the Presidency of the Virginia Tech Faculty Senate.

 ✓ Prof. David G. I. Kingston was recently appointed, by the US Secretary of Health and Human Services, as a member of the National Advisory Council for the National Center for Complementary and Alternative Medicine (NCCAM) for the period 2010-2014. The Council advises the NCCAM Director on research activities and reviews grant applications to the Center. The council comprises 18
regular members, plus the 5 ex-officio members who are leaders of various Federal agencies.

- Prof. Timothy E. Long was named Associate Dean for Strategic Initiatives in the College of Science. Dr. Long is responsible for catalyzing new educational, research, and outreach programs with a focus on promoting interdisciplinary collaborations across the college and university. He will work with research institutes, departments, faculty, and other colleges to develop interdisciplinary initiatives. The 50% administrative appointment will enable Dr. Long to maintain his highly active research program in the Chemistry Department.

- Prof. Judy S. Riffle was named a Fellow of the American Chemical Society Polymer Division. POLY is the second division (after PMSE) to have bestowed this title upon Dr. Riffle. The award recognizes her many contributions to research and education in polymer science, as well as her long record of service to the Division.

- Professor Robert B. Moore was named Interim Associate Director of the Institute for Critical Technologies and Applied Science (ICTAS). Dr. Moore will serve as chief technical officer and advisor to the Institute's director and will share with him responsibilities for technical administration, setting strategic directions and allocating resources on behalf of the institute.

- Prof. Diego Troya was elected to the University Commission on Equal Opportunity and Diversity (CEOD). The CEOD is one of the 7 commissions on campus that play essential roles in University governance.

- Prof. David Kingston continues to serve the National Institute of Complementary and Alternative Medicine, National Institutes of Health, (NCCAM) Board of Scientific Advisors.

- Profs. Tim Long, Bob Moore, Richard Turner, Judy Riffle, Theresa Reineke, Richey Davis (ChemE), and Donald Baird (ChemE) are serving as co-chairs for the 2012 IUPAC World Polymer Conference Organizational Committee—to be held at Virginia Tech in Summer 2012. The meeting is likely to attract upwards of 1200 participants.

- Prof Gordon Yee received the 2010 Alan F. Clifford Faculty Service Award.

- In his role as associate chair, Prof. Herve Marand rewrote all billing procedures for all seven Departmental Service Centers in response to requests by the University Audit Team. The new billing procedures have resulted in invoices being sent to customers of these Service Centers in less than 30 days after services are rendered, in line with University regulations. In past years, invoices were often 2 to 4 months late!

- Profs. Mike Berg and Patricia Amateis served on the University Pre-Med Committee, which required them to interview Virginia Tech students interested in attending medical schools. Interviews consisted of a review of the applicant’s folder and interviewing for approximately one hour and then deciding on the level of recommendation the committee would endorse.

- Prof. Paul Deck organized and managed the 2010 Orientation Week for entering graduate students, including individual advising of all entering students on
entrance test results and initial course plans. He was also responsible for maintaining the department’s website.

✓ Dr. Richard Turner, Director of the Macromolecules and Interfaces Institute, led the MII through VT Commission on Research Five Year Review, with the MII passing with extremely high marks. Turner also led the MII Associate Directors strategic “retreat” planning for the future with the goal of initiating programs to better integrate graduate students across the disciplines in macromolecular science and engineering. Additionally, Turner worked with VT administration exploring options for MII based on 2010 edict from OVPR to reorganize and downgrade MII from its position as a university wide research center. Developed a detailed proposal to establish a “School of Macromolecular Science and Engineering.”

✓ Dr. Richard Turner organized and led the MII Technical Conference and Review—Fall 2010—Three Conference plenary lectures given by a) VP Corporate Research 3M Company, b) Leading researcher in ion containing polymers, and c) Leading researcher in polymeric materials from sustainable monomers.

✓ Dr. Maggie Bobbitt Bump advised the American Chemical Society Student Affiliates Chemistry Club. She developed a variety of activities to promote student creativity, energy, and collegiality, such as a tour of Eastman Chemical Company in Kingsport, TN.

✓ Dr. Bob Moore became Chair-Elect of the Polymer Chemistry Division of the American Chemical Society, 2010. Dr. Moore was also appointed associate director of ICTAS.

Economic Development Activities and Achievements

✓ Techulon Inc., a life sciences company based in the VT Corporate Research Center, has signed an exclusive license with Virginia Tech Intellectual Properties, Inc., to market a new, traceable DNA delivery platform created to deliver genetic medicine to cells while carrying a beacon so scientists can follow its progress. The licensed theranostic material, so-called because it integrates therapies with diagnostics, was created by Prof. Theresa M. Reineke, and Dr. Joshua Bryson, principal scientist at Techulon.

✓ Dr. David Kingston is actively pursuing the development of a Center for Drug Discovery at VT. The downsizing of major pharmaceutical companies means that much future drug discovery will inevitably be done in collaboration with universities and small biotech companies.

K-12 STEM Programs

• Prof. Harry C. Dorn was an invited workshop speaker at Getting Hands-On with Nanotechnology for K-12. UVA INNOVATION Nanotechnology Workshop: Teaching Nanotechnology within Virginia SOLs, University of Virginia, Charlottesville, VA, February 12, 2011.
Community and Student Engagement:

- Dr. Maggie Bobbitt Bump took undergraduate Organic Chemistry students to perform demonstrations at Floyd, Auburn, and Gilbert Linkous Elementary schools. For example, eight students went to Floyd for the afternoon and worked with 60 5th graders for five hands-on lab activities in chemistry. These students earned extra credit for volunteering.

- 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 come and see a chemistry demonstration and hear about the excitement of chemistry. She has been engaged in this activity for eight years now and finds it to be a good way to continue our outreach to K-12 students. 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 ca. 15 years serving to judge projects in many areas.

- As a component of his NSF Career Award, Prof. Lou Madsen is involved in developing activities to initiate scientific motivations in girls age 6-11. During summer 2010, Rachel Leslie, his undergraduate researcher, and Kacey McCreary, his 1st yr. PhD student, continued work on designing “exploration kits” for young girls. 3 pilot kits are under refinement. These two also worked toward establishing an interactive (forum + resources) website to spread this program and interact with kids and parents. Rachel and Kacey are refining the website, and acquired a domain at VT (“www.vt.edu/~playcreatediscover”).

The Department of Chemistry Advisory Council (DCAC)

The previous membership of DCAC was reassessed to identify members that wished to remain active: Frank Akers (chair), Josh Bryson, Elizabeth Calvey, William Coleman, Deanne Emory, Mitch Koppelman, Wayne Ogden, Rob Shenton, Michael Smith, William Starnes, and Dean Webster.

New members of DCAC were appointed:

- Bill Bryant (IMERYS): Ph.D. 2000 with Harry Gibson
- Joe Layman (Albemarle): Ph.D. 1990 with Jim Wolfe
- Tom Piccariello (Synthonics): Ph.D. 1989 with David Kingston
- John Walz: Head of the Chemical Engineering Department at Virginia Tech.
- Michael Borgerding (RJ Reynolds and currently an adjunct professor at Virginia Tech): B.S. 1978, M.S. 1981
- Erick Iezzi (SAIC): Ph.D. 2003 with Harry Dorn
At the Spring DCAC meeting, John Walz (Chemical Engineering) described the mission of that Department’s advisory group, which was embraced by DCAC:

- Give advice and suggestions to Department Head on various matters
- Be an advocate for the Department to the Dean
- Provide confidential feedback to Department Head from meetings with students and faculty
- Provide advice to our students, especially in job seeking
- Serve as external ambassadors for our Department
- Serve as primary donors to the Department

<DCAC photo here>
Department of Chemistry Advisory Council (Spring 2011 meeting)

**DIVERSITY**

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

Each of our faculty members is committed to promoting diversity across the department and within the sciences. In reviewing our efforts over the past year, however, the contributions of Professor Diego Troya warrant special mention. Prof. Troya is a member of Virginia Tech’s Future Faculty Development Program Committee. The program recruits and brings to campus exceptional minority graduate students in all areas who are approximately two years away from applying to academic jobs. Once on campus, the visitors participate in workshops aimed at preparing them for job interviews. Diego is in charge of reviewing all of the applications in Science and some in Engineering (over 30 applications), and selecting qualified individuals among that list. He also participates in organizing the workshop. This initiative is rooted in the AdvanceVT program of the Office of the Provost, and chaired by Peggy Lane. Additionally, Diego was elected to the University Commission on Equal Opportunity and Diversity (CEOD). The CEOD is one of the 7 commissions on campus that play essential roles in University governance. He is also a member of the panel that reviews application to the Women and Minority Scholar and Artist Lecture Series (this year involving 28 applications), which is spearheaded by Ellen Plummer in the Provost Office. Finally, Prof. Troya participated in the interviews for the three finalists for vice president for Diversity and Inclusion (Antonio Farias, Melva Newsom, and William Lewis). Aside from attending the presentations of their plans for Virginia Tech, he visited with them during June and July 2010 as the representative from the Hispanic Caucus.

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

**Specific Diversity Activities, Awards and Honors**

- Dr. Michael A. Berg, Dr. Maggie B. Bump, and Prof. Gary L. Long received 2011
Excellence in Access and Inclusion Awards from Virginia Tech Services for Students with Disabilities. The award is given to members of the VT community for their contributions in enabling disabled students to enjoy the broad range of educational opportunities and services offered within the University.

- Dr. John Morris has been working with the Multicultural Academics Opportunities Program (MAOP) within the university. This involves serving as the principal liaison between the Chemistry Department and the MAOP program, which includes circulating applications to interested chemistry faculty and encouraging them to work with a summer MAOP student.

- Prof. Joseph Merola continues to serve on the College of Science Diversity Committee and contributes to proposal development of a COS diversity initiative.

- Prof. Judy Riffle has engaged in research and recruiting collaborations schools that have high fractions of minority students: She currently has programs funded with St. Paul’s College (HBCU), Lawrenceville, VA, 3 summer 2010 undergraduates plus one Research Experiences for Teachers grant for a teacher from St. Paul’s; University of South Carolina Upstate, key faculty member is Astrid Rosario, 4 summer students under her direction; beginning to work with Virginia State and the University of Puerto Rico at Mayaguez. These programs are coordinated through VA Tech’s Diversity group now headed up by VP William Lewis, but funded by NSF.

- As a female instructor in General Chemistry from a minority ethnic background, Shamindri Arachchige has pursued a variety of outreach activities (VT STARS and Imani Nialah Shadowing Day) benefitting underrepresented and economically disadvantaged students—particular those involving K-12 students in the New River Valley.

- Prof. Jim Tanko was a participant in the 2011 National Diversity Equity Workshop (Open Chemistry Collaborative in Diversity Equity, OXIDE), sponsored by NSF; Arlington, VA January 24 – 26, 2011.

FINANCIAL SUMMARY

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 (CNS, copying, undergraduate laboratories, etc.) Because of increased enrollments, summer school and enrollment support have been steadily increasing. Yet, even this has not been sufficient, and the Department has been forced to use overhead funds to support the education mission. Introduction of lab fees for undergraduate laboratory courses will allow us to discontinue this questionable practice.
Department Finances Summary

<table>
<thead>
<tr>
<th>Income Category</th>
<th>FY-05</th>
<th>FY-06</th>
<th>FY-07</th>
<th>FY-08</th>
<th>FY-09</th>
<th>FY-10</th>
<th>FY-11</th>
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<tbody>
<tr>
<td><strong>208 Base Allocation</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>T&amp;R Faculty Salary</td>
<td>2,835,292</td>
<td>2,919,517</td>
<td>2,881,582</td>
<td>2,850,369</td>
<td>2,901,746</td>
<td>2,912,746</td>
<td>2,982,114</td>
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<tr>
<td>A&amp;P Faculty Salary</td>
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<td></td>
<td></td>
<td></td>
<td>63,000</td>
<td>63,000</td>
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<tr>
<td>Term Faculty</td>
<td>72,606</td>
<td>73,666</td>
<td>77,000</td>
<td>43,476</td>
<td>43,476</td>
<td>43,476</td>
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<tr>
<td>GTA/GA Salary</td>
<td>876,153</td>
<td>907,412</td>
<td>924,048</td>
<td>985,603</td>
<td>903,810</td>
<td>903,810</td>
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<tr>
<td>Staff Salary</td>
<td>836,227</td>
<td>872,354</td>
<td>910,885</td>
<td>958,385</td>
<td>895,385</td>
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<tr>
<td>Operating</td>
<td>335,836</td>
<td>335,836</td>
<td>335,836</td>
<td>333,836</td>
<td>333,836</td>
<td>333,836</td>
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<tr>
<td><strong>Summer School Faculty</strong></td>
<td>126,300</td>
<td>129,200</td>
<td>134,917</td>
<td>196,520</td>
<td>220,653</td>
<td>238,247</td>
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<tr>
<td><strong>Enrollment Support</strong></td>
<td>111,500</td>
<td>106,068</td>
<td>150,963</td>
<td>580,214</td>
<td>712,273</td>
<td>933,169</td>
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<tr>
<td>Faculty Start Up</td>
<td>12,395</td>
<td>216,162</td>
<td>335,498</td>
<td>702,142</td>
<td>476,492</td>
<td>14,526</td>
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<tr>
<td><strong>SCHEV Allocations</strong></td>
<td>167,900</td>
<td>168,000</td>
<td>229,699</td>
<td>237,500</td>
<td>196,051</td>
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<td><strong>Overhead Return</strong></td>
<td>268,925</td>
<td>333,702</td>
<td>288,241</td>
<td>392,905</td>
<td>413,450</td>
<td>425,725</td>
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<td>Virginia Tech Foundation</td>
<td>30,840</td>
<td>4,670</td>
<td>5,680</td>
<td>8,050</td>
<td>6,050</td>
<td>14,000</td>
<td></td>
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<tr>
<td>Friends of Larry Taylor Account</td>
<td>30,508</td>
<td>43,499</td>
<td>23,977</td>
<td>16,895</td>
<td>13,655</td>
<td>29,522</td>
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<tr>
<td><strong>Totals</strong></td>
<td>5,463,976</td>
<td>5,491,026</td>
<td>6,294,992</td>
<td>6,503,296</td>
<td>7,351,772</td>
<td>7,232,326</td>
<td>7,072,861</td>
</tr>
</tbody>
</table>

Stockroom Debt Repayment

A solution to the long-running “Chemistry Stockroom debt” problem was reached, courtesy of the College of Science. The Department will pay approximately $26K/year to the College in payment of a loan to relieve the debt, and pending an acceptable audit of procedures and practices, the College will contribute $50K of its own resources in payment of the debt.

Partnership with Agilent Technologies

Funding through a major loan from the College of Science (> $1M) allowed a major upgrade to our undergraduate laboratories that included purchase of state of the art equipment for non-majors general chemistry (6 gas chromatographs/mass spectrometers, and atomic absorption spectrometer) and non-majors organic (FTIR, GC, HPLC, single quad LC-MS, and a 400 MHz NMR lab). The magnitude of these purchases provided leverage which helped the department negotiate a partnership with a major instrument manufacturer (Agilent Technologies), the benefits of which include significant discounts on the equipment purchased (30%--greater than the normal academic discount of 20%), future donations of equipment to the department for the
undergraduate labs, an instrument loan program for new faculty (free use of equipment for a year, with the option of purchasing afterward with a 37% discount), extended warranties, software loan program, etc. In addition, Agilent will assist with the development and dissemination of new educational material.

**Overhead Funds**

Overhead funds come from sponsored research for the purpose of supporting/enhancing research in the department. The major use of these funds is for start-up of new faculty—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 two years.

**Overhead Account (230405) Expenditures**

<table>
<thead>
<tr>
<th>Expenditures</th>
<th>2010</th>
<th>2011</th>
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</thead>
<tbody>
<tr>
<td>SALARIES</td>
<td>$160,783</td>
<td>$258,480</td>
</tr>
<tr>
<td>GTA/GA</td>
<td>$67,226</td>
<td>$141,360</td>
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<tr>
<td>T&amp;R FACULTY</td>
<td>$24,492</td>
<td>$49,820</td>
</tr>
<tr>
<td>T&amp;R INSTRUC</td>
<td>$1,327</td>
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<tr>
<td>POST-DOCS</td>
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<td>$20,357</td>
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<td>SUMM SCHL FAC</td>
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<tr>
<td>STAFF</td>
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<td>$10,950</td>
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<tr>
<td>WAGES</td>
<td></td>
<td>$10,378</td>
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<tr>
<td>FRINGES</td>
<td>$15,683</td>
<td>$25,615</td>
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<tr>
<td>ADMIN</td>
<td>$86,952</td>
<td>$126,263</td>
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<tr>
<td>ADMMIS</td>
<td>$7,333</td>
<td>$3,034</td>
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<tr>
<td>BLDGMT</td>
<td>$9,374</td>
<td>$4,349</td>
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<tr>
<td>BLDGRN</td>
<td>$3,306</td>
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<tr>
<td>CHAIRS</td>
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<td>$26,627</td>
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<tr>
<td>COPIER</td>
<td>$2,614</td>
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<tr>
<td>DELSRV</td>
<td>$88</td>
<td>$114</td>
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<tr>
<td>FCRUT</td>
<td>$21</td>
<td>$12,246</td>
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<td>GROTOVR</td>
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<td>$163</td>
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<tr>
<td>GRUTFND</td>
<td>$43,851</td>
<td>$4,700</td>
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<td>OFCOP</td>
<td>$6,614</td>
<td>$633</td>
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<td>RSKMGT</td>
<td>$13,751</td>
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<td>ALUMNI</td>
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<td>FSETUP</td>
<td>$19,409</td>
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<td>GRPPROG</td>
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<td>OhIoPI</td>
<td>$40,086</td>
<td>$48,259</td>
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<td>SRVCTR</td>
<td>$1,574</td>
<td>$3,669</td>
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<tr>
<td>UGLABS</td>
<td>$24,587</td>
<td>$43,643</td>
</tr>
</tbody>
</table>
As noted, the Department successfully recruited two new faculty members this year. Our startup package was clearly competitive, and we were able to achieve this without mortgaging the future, mainly because of the surplus that this administration inherited (three years without hiring), in addition to support from the College and Provost (including additional special opportunity funding from the latter).

Nonetheless, various challenges are on the horizon. Generally, the Provost’s Office caps their 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 including continued brinksmanship in terms of a budget deal, government shutdown, and debt ceiling limit 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 & sustain research.

Over the course of the next academic year, the Department will engage in a philosophical discussion about the proper use of overhead funds, and address issues such as:

- What activities are/are not appropriate uses of overhead funds?
- Should faculty who lose funding be provided with bridge funding from overhead? With what limitations?
- What is our commitment to graduate students we admit?
- What are the expectations of faculty members receiving departmental support for research (submitted proposals, etc.)?
- Should some portion of overhead be returned PIs?

**Discretionary Funds**

We have been extremely concerned about discretionary funds (foundation account) available to the Department. These funds are used to the Highlands in Chemistry colloquium program, faculty recruiting, graduate and undergraduate student recruiting, K-12 outreach, 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:

<table>
<thead>
<tr>
<th>UGPROG</th>
<th>$609</th>
<th>$862</th>
</tr>
</thead>
<tbody>
<tr>
<td>TOTALS</td>
<td>$368,131</td>
<td>$501,852</td>
</tr>
</tbody>
</table>

Status of the Chemistry VT Foundation Accounts:
Friends of Larry Taylor Endowed Account (886047) as of 06/01/11:

- Carry-over from FY 2010: $49,619.28
- Gifts in FY 2011: $7,350.00
- Unrealized+Realized Gains/Losses: $8,022.63
- Income: ($1,690.56)
- Fees (Management/Administration/Assessment): ($1,131.51)
- Endowment as of 06/01/11: $62,169.84

Friends of Larry Taylor Income Account (873172) as of 06/01/11:

- Carry-over from FY 2010: $8,893.86
- Income in FY 2011: $2,115.03
- Expenses in FY 2011: $0.00
- Income Account Balance (873172) as of 06/01/11: $11,008.89

Chemistry General Account (881327) as of 06/01/11:

- Carry-over from FY 2010: $133,730.56
- Gifts in FY 2011 as of 06/01/11: $29,522.50
- Other revenues as of 06/01/11: $3,631.63
- Expenses in FY 2011 as of 06/01/11: $34,673.08
- Account Balance as of 06/01/11: $132,211.61

Distribution of Expenditures of VTF funds (881327) for FY 2011:

<table>
<thead>
<tr>
<th>Activity</th>
<th>Amount</th>
<th>Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>Alumni Newsletter and Chemistry Advisory Council</td>
<td>$11,415</td>
<td>32.9%</td>
</tr>
<tr>
<td>Activities</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Faculty, Staff and Student Awards</td>
<td>$6,085</td>
<td>17.5%</td>
</tr>
<tr>
<td>Graduate Recruiting</td>
<td>$4,599</td>
<td>13.3%</td>
</tr>
<tr>
<td>Departmental Activities for Grad./Und. Students/Staff/Faculty</td>
<td>$2,825</td>
<td>8.1%</td>
</tr>
<tr>
<td>Faculty Recruiting</td>
<td>$2,565</td>
<td>7.4%</td>
</tr>
<tr>
<td>Gift Assessment Fees paid to VTF</td>
<td>$1,925</td>
<td>5.6%</td>
</tr>
<tr>
<td>OSP Transfers</td>
<td>$1,314</td>
<td>3.8%</td>
</tr>
<tr>
<td>Seminar Program</td>
<td>$1,305</td>
<td>3.8%</td>
</tr>
<tr>
<td>Undergraduate Recruiting</td>
<td>$797</td>
<td>2.3%</td>
</tr>
<tr>
<td>K-12 Outreach</td>
<td>$566</td>
<td>1.6%</td>
</tr>
<tr>
<td>Commencement Activities</td>
<td>$200</td>
<td>0.6%</td>
</tr>
<tr>
<td>Miscellaneous</td>
<td>$1,077</td>
<td>3.1%</td>
</tr>
</tbody>
</table>
Since about 2005, the balance available to the Department has been decreasing by about $40K/year, which would mean the money for these activities would cease to be available by ca. 2014.

The problem seems to be a decline in the amount of gifts to the department over the past few years. The following plot shows gifts received by the department over the past few years. (Note: Royalties from lab manuals, DVD sales, etc. were omitted from this plot):
To address this problem, several actions were taken:

- 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) was published in November 2010 after an approximately 2½ year hiatus, with a Spring 2011 edition currently in press. The intent is to continue publishing this newsletter near the end of each Fall and Spring semester (as long as funding permits).
- The Department of Chemistry Advisory Council was reinvigorated. Successful and productive meetings were held in November 2010 and April 2011. At the April meeting, DCAC revisited its mission, and began to develop a plan to assist the Department on various fronts.

Only time will tell whether the apparent uptick in the balance observed 2010–11 can be attributed to the success of these initiatives.

Finally, the following table summarizes research related expenditures for FY06 – present.

<table>
<thead>
<tr>
<th></th>
<th>FY06</th>
<th>FY07</th>
<th>FY08</th>
<th>FY09</th>
<th>FY10</th>
<th>FY11</th>
</tr>
</thead>
<tbody>
<tr>
<td>Res Outputs</td>
<td>(YTD)</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ttl OH</td>
<td>$1,264,125</td>
<td>$1,165,185</td>
<td>$1,160,156</td>
<td>$1,764,325</td>
<td>$2,095,120</td>
<td>$1,896,617</td>
</tr>
<tr>
<td>Res Expenditures</td>
<td>$6,441,831</td>
<td>$7,802,964</td>
<td>$6,879,104</td>
<td>$9,529,122</td>
<td>$9,795,089</td>
<td>$8,510,415</td>
</tr>
<tr>
<td>Eff OH Percent</td>
<td>24.4%</td>
<td>17.6%</td>
<td>20.3%</td>
<td>22.7%</td>
<td>27.2%</td>
<td>28.7%</td>
</tr>
<tr>
<td>Res Awards ($)</td>
<td>$8,344,140</td>
<td>$6,167,921</td>
<td>$13,024,140</td>
<td>$11,416,151</td>
<td>$12,328,066</td>
<td>$6,441,293</td>
</tr>
<tr>
<td>Res Awards (#)</td>
<td>59</td>
<td>67</td>
<td>83</td>
<td>83</td>
<td>76</td>
<td>63</td>
</tr>
<tr>
<td>Total GS</td>
<td>110</td>
<td>113</td>
<td>119</td>
<td>130</td>
<td>128</td>
<td>138</td>
</tr>
<tr>
<td>Payroll</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>GRA</td>
<td>$933,255</td>
<td>$732,985</td>
<td>$905,400</td>
<td>$1,089,399</td>
<td>$932,121</td>
<td>$896,420</td>
</tr>
<tr>
<td>GTA</td>
<td>$1,051,174</td>
<td>$1,200,743</td>
<td>$1,331,855</td>
<td>$1,367,714</td>
<td>$1,454,250</td>
<td>$1,639,935</td>
</tr>
<tr>
<td>Ratio (RA / TA)</td>
<td>0.89</td>
<td>0.61</td>
<td>0.68</td>
<td>0.80</td>
<td>0.64</td>
<td>0.55</td>
</tr>
<tr>
<td>Enrollment (PhD &amp; MS)</td>
<td>124</td>
<td>120</td>
<td>128</td>
<td>141</td>
<td>148</td>
<td>155</td>
</tr>
</tbody>
</table>