

**Chemistry Department**  
**Annual Report**  
**July 1, 2004 – June 16, 2005**

The Chemistry Department is in good health despite an inadequate resource base resulting from state budget cuts in 2001-2002. With a restoration of base funding and further investment to bring the department to adequate funding levels, the Chemistry Department is poised to reach new heights of excellence. To begin with a highlight that is a clear indicator of the department's determination to progress even under adverse conditions, the department saw an increase in NSF research expenditure rankings from 53<sup>rd</sup> to 39<sup>th</sup> even as it was experiencing the state mandated budget cuts. This is a testament to the quality and determination of the chemistry faculty. In addition, Virginia Tech data indicate that the Chemistry Department is the third highest rated department in terms of grant awards behind two engineering departments that have twice the faculty of the Chemistry Department and without the high service teaching load that Chemistry has.

The following sections give further information about the accomplishments of the department during the past fiscal year.

**Research:** The Chemistry Department added Dr. Diego Troya to a tenure track position. Dr. Troya is a computational chemist and his position is part of the computational science cluster hiring initiative in the College of Science. Within the Chemistry Department we now have two computational chemists, Dr. Troya and Dr. T. Daniel Crawford. Renovations underway in the Department will provide controlled environment space for up to 200 computers in two or more clusters for computational work. Drs. Troya and Crawford have a total of 6 graduate students, 8 undergraduates, and 1 postdoctoral fellow working on theoretical chemistry projects that range from materials chemistry to fundamental properties of chiral molecules of pharmacological significance. There is still a need within the Department for a computational chemist with expertise in biomacromolecular chemistry. Such a person would interact well not only with the computational cluster but also the structural biology cluster.

Dr. Sungsool Wi joined the Department as a Visiting Assistant Professor. Dr. Wi's appointment was made as a result of the nanoscience cluster search in FY2004. It is the Chemistry Department's wish that Dr. Wi's appointment be converted to a tenure track position as soon as possible. Indeed, it is the Department's understanding that the conversion will take place with the first available retirement in the Department. We note that Dr. Viers retires this summer therefore we expect that Dr. Wi will be appointed to a tenure track position concomitant with Dr. Viers' retirement.

In FY2005 the Department participated again in the College of Science cluster hire initiatives. These searches are ongoing. The department was not successful in recruiting Dr. Ken Wagener of the University of Florida. Dr. Wagener would have joined the Macro program with an appointment in the Chemistry Department. Dr. Wagener indicated that he may be interested at some future time in moving to Virginia

Tech but at the present time such a move did not make sense for him. The Chemistry Department has identified two senior level people, Dr. Nicole Sampson and Dr. Peter Tong both of Stonybrook, who are interested in moving their research programs. Drs. Tong and Sampson will be a significant catch for the University that successfully recruits them.

The Department is also taking advantage of opportunity hires to increase the expertise and research base of the department in areas of identified need. Dr. Daniel Capelluto, spouse of a Biology hire, will be joining the department this summer as a Research Assistant Professor in the area of protein chemistry. His addition will complement the work of Sungsool Wi quite nicely. In addition, Dr. Cathy Sarisky, spouse of a professor at Radford University, will also join the department as an adjunct professor and her area is also protein chemistry.

The Chemistry Department actively pursues extramural funding for research. There is an increasingly competitive environment nationally for basic research funding and, in Chemistry we find that the success rate for proposals is lower than in previous years. Through May in FY 2005 the Department added \$4.2M in new funding. This is down slightly from last year but leads the College of Science. The Chemistry Department has \$9.4 M in active funding. Two NSF funded IGERT programs are headed by faculty in Chemistry. Dr. Riffle directs an IGERT entitled "Macromolecular Science and Infrastructure Engineering," and Dr. Timothy Long co-directs an IGERT, "Macromolecular Interfaces with Life Sciences" (MILES.) Dr. Dorn continues to run a Nanotechnology Undergraduate Education Program funded by NSF and Dr. Anderson directs an NSF funded Research Experience for Undergraduates Program. The Chemistry Department at Virginia Tech is the lead Department for a Department of Defense MURI award on "Macromolecular Architecture for Performance;" the other institutional participants are Cornell and Penn State.

Chemistry faculty serve on the editorial boards of eight journals and serve on nine national society committees. The Chemistry faculty published 112 articles in refereed journals, 26 reviews and book chapters, three books, and received eight patents in the calendar year 2004.

**Graduate Education:** The Chemistry Graduate program had 112 students pursuing advanced degrees in Chemistry during the 2004-2005 academic year. In addition, 25 students pursuing graduate degrees in other disciplines (e.g. MACRO) conduct their dissertation research in the laboratories of Chemistry faculty. Of the 112 students, 25 began their graduate studies during the fall 2004 semester. 4% of the current graduate student population are African American and 37% are women. Recruiting efforts during the spring 2005 semester focused on increasing the diversity and the size of the graduate student population, in concert with the goals of the PhD 2010 initiative. A total of 31 students accepted our offer of admission (an increase of 20% over previous year's recruiting totals). Of these, three students are African American, 1 is Hispanic, and 16 are female. The department was successful in attracting a very good applicant pool, and we anticipate that the entering class for fall 2005 will be a strong group of students. This

is reflected in the awarding of a Cunningham fellowship, a Dean's Diversity Assistantship, and two PhD 2010 Assistantships to four of the entering students.

The Chemistry Department also conducted its five year assessment of the Graduate program. Alumni that responded to our questionnaire were happy with their graduate education and the career opportunities that it afforded. In response to our survey, Alumni and prospective employers suggested the importance of a broad based educational experience. Alumni felt that our program offered good exposure to interdisciplinary research activities, but suggested that exposure to areas outside of chemistry (such as business) might be beneficial.

During the five years that the assessment covered, the average time to PhD was just over 5 years. Several changes to the curriculum had been implemented between 2001 and 2003 that were intended to help shorten the time to degree. The success of these changes, we believe, will not be fully apparent until the next assessment. Of these changes, the formal Literature Review course, and the Original Research Proposal course give students an opportunity to write and critically evaluate the literature within the context of their research area – and helps the students organize and write their dissertation beginning at an earlier stage of their graduate studies.

Nine students earned a PhD in Chemistry and four students earned a MS in Chemistry during the 2004-2005 academic year. These numbers are consistent with previous years.

**Undergraduate Education:** The number of chemistry majors remains steady and healthy at approximately 200. Record numbers of students presented at the departmental Undergraduate Research symposia during 2004-05, indicating that the students are reaching a high level of achievement. The recently completed five-year outcomes assessment indicates that alumni appear to be very satisfied with the chemistry program and with the quality of instruction by the chemistry faculty. Assessment of individual courses was obtained from senior exit interviews conducted during Spring 2004. Overall the senior interviews are consistent with the alumni survey: students view the quality of instruction and their interactions with the Chemistry Department faculty very favorably. The core courses in our baccalaureate program; general, organic, and physical chemistry; and the faculty members who teach these courses are rated highly. Even conceptually difficult courses are appreciated for the knowledge learned. Most critical comments are directed at the workload for low-credit labs or courses, which has increased with the requirement for writing-intensive courses, and with class size or composition.

Service Student Credit Hours continue to be greater than 80% in the Department of Chemistry and the imbalance between the fall and spring semesters presents additional challenges. Enrollments in most lower-level chemistry classes continue to increase gradually. General Chemistry lab was oversubscribed by 200 students during Fall 2004 leading to some overcrowding in the laboratories. Greater scheduling efficiency as a result of eliminating the 1074 General Chemistry for Engineers course will reduce this number to 50-100 in the upcoming year.

The most significant change in the undergraduate program during 2004-05 was the completion of moving all laboratories to the new Chem-Phys building. These new facilities have a huge impact on the morale of our current students, and, based on anecdotal feedback from prospective students, on student recruiting.

Goals for Undergraduate Education: The two major goals for the next few years are to upgrade the laboratory curriculum to match the new facilities and to better coordinate the overall chemistry curriculum. We believe that a chemistry graduate, given a "chemical" problem, should be able to:

1. research the problem
2. develop an approach to solve the problem, including designing experiments to test the approach and revising the approach based on new data (repeating as necessary)
3. reach conclusions weighing the pros and cons of the results and state uncertainty/risks correctly
4. pursue this work in a team if appropriate and be able to communicate well (both 1-way and 2-way)

To help students reach these competencies we will make the following changes in our curriculum.

#### 1000-level classes

Develop independent-learning skills, i.e., the ability to learn from a textbook; develop problem-solving skills and begin the transition from algorithmic problem solving to conceptual understanding.

#### 2000-level

Begin to "chunk" information and apply concepts in new applications.

#### 3000-level

Synthesis of concepts to form new ideas

#### 4000-level

Demonstrate creativity and original thinking in completing tasks.

**Service and Outreach:** The ChemKit program directed by Professor Gary Long continued to serve the Commonwealth during 2004-05. The project supplied experiments on Conductivity, Water analysis (Hach Kits), Solubility, Stoichiometry, TLC, and Vitamin C. There were several thousand Student-Conducted Experiments at ~30 schools. During the course of the Mobile Chemistry Lab and ChemKit outreach programs, more than sixty teachers were trained in basic and/or advanced workshops since 2001. Funding of the ChemKit program ends this year and no substitute funding has been found to continue the program.

A group of teachers from Roanoke Valley Governor's School (<http://rvgs.k12.va.us/>) visited campus on March 7 to learn how they might incorporate nanotechnology into their

curriculum. Carla Slebodnick provided a tour of the crystallography lab and brought the group to ChemPhys. Several chemistry faculty gave short presentations:

- Brian Tissue (luminescent nanoparticles)
- Alan Esker (POSS nanostructures)
- Diego Troya (computational chemistry applied to nanoscience)

The teachers toured Hahn 005, which houses John Morris's surface analytical instruments and Brian Tissue's nanoparticle synthesis chamber.



Graduate student Larry Fiegland describes the analysis chamber for in-situ infrared and surface spectroscopy to Cindy Bohland, Cam Srpan, John Kowalski, and Steve Smith. In the background graduate student Wes Gordon shows a nanoparticle synthesis chamber to Shewaferaw Shibeshi. Also attending, but out of the picture, were: Fred Hoffman, Walker Holt, and Gwen Sibert.

**Alumni Development:** Several of our recent graduates were recognized for their accomplishments this past year. Notable was Dr. William Bryant (Ph.D. 1999) who received the Virginia Tech College of Science Young Alumni Award.

Our alumni advisory counsel continues to be very active. A total of 29 alumni sit on the council, at the fall meeting of 2004, 14 alumni attended and in the spring of 2005 we had 12 members of the council in attendance. The spring meeting of the council was held to coincide with our undergraduate research symposium to give our alumni a chance to interact with our juniors and seniors. Our commencement speaker for 2005 was Mr. Scott Banks (B.A. Chemistry 1981).

Giving to the Department has added significantly to several scholarship endowments. Please see the Appendices.

## Appendix 1.

### **Undergraduate Education**

Awards and other noted achievements of undergraduate students

Academic Excellence Award: **Adrian Campbell, Jeffrey Carter, Matthew Hunley, and Charlie Thomas**

American Institute of Chemists Award: **Robert Schmidt**

James Lewis Howe Award (presented by the Virginia Blue Ridge Section of the American Chemical Society): **Veronica Pugh**

Hypercube Scholar Award: **Jeffrey Carter**

The Merck Index Award: **Jennifer Loman**

Phi Lambda Upsilon Award: **Charlie Thomas**

Undergraduate Research Award: **Sarah Huffer, Matthew Jeletic, and Miriam Konate**

Analytical Chemistry Award: **Paul Williams**

CRC Freshman Chemistry Achievement Award: **Stephanie Moore**

Viers Achievement Award: **Katherine Howell and Tyler Luong**

**Matthew Shoulders** was awarded a Department of Homeland Security undergraduate scholarship for the 2003-2004 academic year. This is the first year the scholarship has been offered. The scholarship provides for tuition and fees and a monthly stipend until he graduates in the spring and also entails an eight to ten week internship in the summer of 2004 at a site selected by the Department of Homeland Security. Matthew is a BS chemist in the Virginia Tech Department of Chemistry. He is advised by Prof. Felicia Etzkorn.

### Names of students participating in undergraduate research

(Undergraduate students in bold)

Fall 2004 Undergraduate Research Symposium

December 3, 2004

"Reisert Compounds in Asymmetric Synthesis." **Monty Hayes** and H. W. Gibson. Department of Chemistry, Virginia Tech.

"Light Activated DNA Interactions of Supramolecular Complexes." **Jerita Dubash**, Matt Mongelli, Karen Brewer. Departments of Chemistry and Biology, Virginia Tech.

"Synthesis and Characterization of [(tpy)Os(dpp)Cl]PF<sub>6</sub>." **Matt Jeletic**, Karen Brewer. Departments of Chemistry and Biology, Virginia Tech.

"Synthesis of Tri-headed amphiphiles for the creation of a topical microbicide." **Erika Bechtold**, and Richard Gandour. Departments of Chemistry, Virginia Tech

"Arylation of Cyclopentadienes Using Organochromium Reagents." **Mariam M. Konate** and Paul A. Deck. Department of Chemistry, Virginia Tech.

"Perfluorotolyl-Substituted Cyclopentadienes." **Benjamin D. McCauley** and Paul A. Deck. Department of Chemistry, Virginia Tech.

"Electrospinning Polyelectrolytes and Block Copolymers." **Matthew T. Hunley**, Matthew G. McKee, and Timothy E. Long. Department of Chemistry, Virginia Tech.

Spring 2005 Undergraduate Research Symposium

April 29, 2005

"Synthesis of surfactants for use as microbicides." **Erika Bechtold** and Richard Gandour. Department of Chemistry, Virginia Tech.

"Synthesis of a Ser-cis-Pro Alkene Isostere." **David May** and F. Etzkorn. Department of Chemistry, Virginia Tech.

"pH Effects on Trisilanolphenyl-POSS Stability." **Sarah M. Huffer**, Alan R. Esker, Kevin J. Dawson, Jianjun Deng. Departments of Chemistry and Chemical Engineering, Virginia Tech.

"Interplay of Phase separation and dewetting in filled poly t-butyl acrylate films as a function of temperature." **Michael Swift**, Alan R. Esker, Ritu Paul. Department of Chemistry, Virginia Tech.

"Ab Initio Prediction of Optical Rotation in (1S,5S)-beta-Pinene." **Adel Ghaderi** and T. Daniel Crawford. Department of Chemistry, Virginia Tech.

"Synthesis of a Biosensor Using Fluorescent Proteins to Cadmium in an Aqueous System." **Alison Smith**, Michael Hochella, Brenda Winkel, and Brian Lower. Departments of Biology and Geosciences, Virginia Tech and Pacific Northwest National Lab.

"Using 31P NMR and a phosphine tag to monitor stereochemistry and reactivity of Ru(II) light absorbing units in supramolecular assemblies." **Julie Heinecke** and Karen J. Brewer. Department of Chemistry, Virginia Tech.

"Synthesis of di-2-hydroxyethyl dicyanofumarate." **Mary Spencer**, Bill Tyree, Guangbin Wang, Carla Slebodnick, and Gordon T. Yee. Department of Chemistry, Virginia Tech.

"Theoretical Calculations of Optical Rotation in the Flexible Molecule (R)-Limonene." **Jeffrey E. Carter** and T. Daniel Crawford. Department of Chemistry, Virginia Tech.

"Synthesis and characterization of highly branched, biodegradable, poly(caprolactone) containing polyurethanes." **Kristin Sisson** and Timothy E. Long. Department of Chemistry, Virginia Tech.

"The Influence of Intermolecular Interactions on the Formation of Functional Fibers." **Matthew Hunley**, Matthew G. McKee and Dr. Timothy E. Long. Departments of Chemical Engineering and Chemistry, Virginia Tech.

## Appendix 2

### Highlights from 2004.

- **Brian Tissue** served as a program director in the NSF Division of Chemistry from Sept 04 through Dec 05.
- The 2004 winner of the Flory Education Award presented by the Division of Polymer Chemistry of the ACS is the team of **Prof. Jim McGrath, Prof. Garth Wilkes** and **Prof. Tom Ward**.
- **Prof. Daniel Crawford** gave an invited lecture in July 2004 at Cambridge University, entitled "Molecular Quantum Mechanics". The meeting was held in honor of Prof. Nicholas C. Handy, a pioneer in electronic structure methods. Daniel was one of 25 invited speakers.
- **Prof. Tim Long** has been listed as a winner in the FY 2004 competition under the Defense University Research Instrumentation Program (DURIP). The Department of Defense announced plans to award \$43.5 million to academic institutions to support the purchase of research instrumentation.
- **Prof. Tim Long** presented an invited lecture dealing with recent advances in real-time reaction monitoring using mid-infrared spectroscopy. The International Union of Pure and Applied Chemistry (IUPAC) Conference was held in Paris, France from July 4-9, 2004 and was attended by nearly 3000 participants, including several plenary lectures by Nobel Laureates including Jean Marie Lehn in the area of supermolecular structure. Prof. Long's presentation described recent efforts in stable free radical polymerization, polyurethane synthesis, and the formation of stable phosphorous containing nitroxides.

## Appendix 3

### **Annual Statistical Information:**

#### Summary of Research and Related Scholarly Activities

Articles in Refereed Journals	112
Presentations at Professional Meetings	56
*Invited Lectures (Off-campus)	43
Research Funding	9.4 million
Books and Monographs	3
Patents	8
Review Articles and Book Chapters	26
Memberships on Journal Editorial Boards	8
Memberships on National Committees	9
Short Courses Taught	18
Students pursued Masters & Ph.D. degrees in 2004-2005 academic year	112
Students received Ph.D. degrees during the 2004-2005 academic year	9
Students received M.S. degrees during the 2004-2005 academic year	4
Students received BA/BS degrees during the 2004-2005 academic year	31

\*Does not include invited presentations at professional meetings, which are included in the previous category.

## Appendix 4

## Chemistry Endowments

Fund	March 2004	May 2005
Hopper Harvie Endowment	25,911	26,641
Chemistry Friends Scholarship	91,338	102,569
Keyser Chemistry Endowment	28,846	29,659
Walker Scholarship	27,818	28,602
Bilisoly Scholarship	108,540	111,599
McNair Fund Endowment	8,273	9,017
Dallas Kinser and R. T. Johnson	29,161	33,502
McGrath Professorship Endowment	9,300	44,468
J. P. Wightman Scholarship <sup>a</sup>	33,939	36,280
John Dillard Scholarship <sup>a</sup>	16,252	112,917
TOTAL	\$379,378	\$535,254

<sup>a</sup> Administered by the Center for Adhesive and Sealant Science now MII (these are included because they recognize Chemistry Faculty)