

ELEMENTS

The Alumni Magazine of the Department of Chemistry at Virginia Tech - Spring 2011



From the Department

Dr. James Tanko

As of this writing, we are in the final days of the

Advanced Analytical Chemistry in the fall semester.

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. I believe 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. Starting this fall, our 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.

So, what about the renovation of Davidson Hall? Although the final word has not yet been received, all indications are that this will likely begin

Continued on Page 2

What's Inside:

Alumni Spotlight 3

Awards 5

Student News 6

Faculty Spotlight 7

Alumni News 9

Chemistry News 11

Staff Spotlight 13

Donors 15



Tel: 540-231-6687
Fax: 540-231-3255
jtanko@vt.edu
www.chem.vt.edu

Spring 2011 semester. Final exams have begun, and we are about a week from graduation day. This small contribution to Elements provides a nice opportunity to reflect on all that has happened in the Department of Chemistry this academic year.

For the first time in three years we were in a position to hire new faculty members, and were 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 post-doctoral 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 nano-scale, ordered scaffolds for tissue engineering and drug delivery. She will be teaching Ad-

Department Chair *(Continued from Page 1)*

early in the fall. 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 \$2,000,000—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, but the final plan is not yet in place. Thus, although the "word" has not yet been given, an awful lot of money and time is being invested. Given the state of resources at the university, it seems unlikely that all of this would be happening if the plug were going to be pulled on the project. 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!

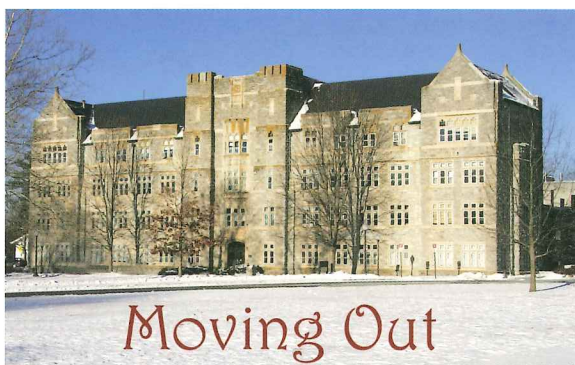
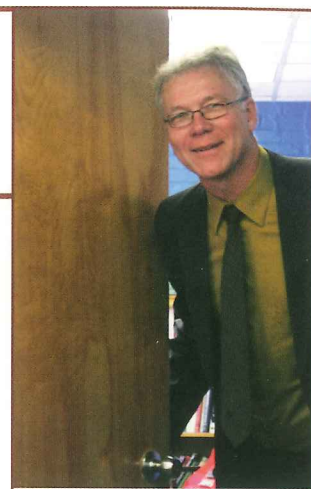
The Department of Chemistry Advisory Council (DCAC) held its Spring meeting in April. The timing proved fortuitous because this meeting coincided with our Research Expo (undergraduate poster session) and the Undergraduate Research Symposium (undergraduate research talks). In

fact, DCAC members were recruited to serve as judges to award prizes for the best undergraduate poster/presentation. Later that evening, DCAC members were treated to the Chemistry Department Awards Ceremony, where we acknowledge the outstanding achievements of our students. The business meetings were exciting and energetic, and DCAC is poised to help move the Chemistry Department towards a bright and exciting future. While on this topic, it would

be appropriate to welcome the new DCAC members: Michael Borgerding, Bill Bryant, Josh Bryson, Chris Curfman, Erick Iezzi, Joe Layman, Tom Picariello, and John Walz. Continuing to serve are Frank Akers (chair of DCAC), Beth Calvey, Bill Coleman,

Deanne Emory, Mitch Koppelman, Wayne Ogden, Rob Shenton, Mike Smith, Bill Starnes, Joe Thrasher, and Dean Webster. The efforts of all these individuals for the benefit of our student, faculty, and program are sincerely appreciated.

Unfortunately, not all the news is good. Mary Jane Altizer, who served the university for 20+ years recently passed away. I fondly remember Mary Jane, as she was near our first lab in Davidson (working as a secretary for Jim Wightman at the time). Finally, we are also sad to report that Theresa Reineke will be leaving at the end of this academic year to join the faculty in the chemistry department at the University of Minnesota. This move will allow her to be in closer proximity to her family, and we wish her the absolute best in the future.



John Walz, Wayne Ogden, Bill Coleman, Beth Calvey, Tom Picariello, Bill Bryant, Joe Thrasher and Joe Layman



Alumni Spotlight

Joseph S. Thrasher

(B.S., 1978; Ph.D., 1981, Inorganic Chemistry)

Coming Full Circle – Almost

Many of you may not realize, but I was supposedly the first Virginia Tech chemistry major allowed by the Graduate Committee to stay on for my Ph.D. degree, and I was also Prof. Alan Clifford's last Ph.D. student. Those of you from the same timeframe in the Department might remember that my wife Debbie worked as a lab technician in Dr. McGrath's group (We are pictured below in the office area of the Clifford laboratory, Room 125 Davidson Hall back in the early 1980s next to a more recent photograph from 2011).

As things turned out, I kept up my end of the agreement with the Graduate Committee, as Debbie and I headed off to my foreign postdoctoral research stay in West Berlin, Germany in November 1981. We have no regrets of our decision as Debbie and I traveled as much as time and money would allow, while I was able to have both a very meaningful and productive research experience. On one trip, we were joined on that trip by another Virginia Tech (and Clifford) alumnus Dr. Jon Howell (Ph.D., 1979) and his first wife Evelyn.

After spending almost two years in Berlin, we returned to the States where I took a visiting assistant professor of chemistry position at Clemson University for the 1983-84 academic year. We headed further

south the next year to The University of Alabama, where I began my independent academic career, and shortly thereafter Debbie got a staff position in the University's Purchasing Department. I rose through the academic ranks at Alabama and served as Director of Graduate Studies (1995-2002) for seven years as well as Department Chair for five years (2002-2007). I was also blessed to have recruited another Virginia Tech alumnus in Dr. Matthew Clark (B.S., 1984) as my first graduate student at Alabama.

Our research has remained in the field of fluorine chemistry, and in recent years it has focused on (1) sulfur-fluorine chemistry, (2) industrial fluorine chemistry, and (3) fuel cell technology. Significant accomplishments have included the synthesis and characterization of $(\text{SF}_5)_3\text{N}$ and SF_5NO_2 in the first area, while research with the chemical industry began with process development work on CFC alternatives and more recently has dealt with either agrochemical or pharmaceutical intermediates. In the area of fuel cell technology, our research focuses on the preparation of improved polymer electrolyte membranes, and we have one of the few academic laboratories that can safely handle 100+-gram quantities of tetrafluoro-ethylene (TFE). On the home front, we opted never to have children; however, we did have some four-legged critters

of the Shetland sheepdog bred, but Brandy, Twister, and Katie are no longer with us except in memory and spirit.

This summer, after 27 years of service both Debbie and I will retire from The University of Alabama, and I have accepted the position of Professor of Chemistry at Clemson University beginning August 15, 2011. At Clemson, it will be my distinct pleasure and honor to overlap with and then follow Prof. Darryl DesMarteau in the area of fluorine chemistry; I will forever be grateful that the majority of the chemistry faculty at Clemson had the foresight to try to maintain an area of chemistry that Prof. DesMarteau has built there over the last ca. 30 years.

I realize that I have big shoes to fill in Clemson; however, excellent facilities should give us a good chance to be very productive. In addition to state-of-the-art research laboratories at the Advanced Materials Research Laboratory (AMRL) in Clemson's Research Park near I-85 in Anderson, South Carolina, we will have an improved barricade facility for TFE work as well as high-bay space for pilot plant projects.



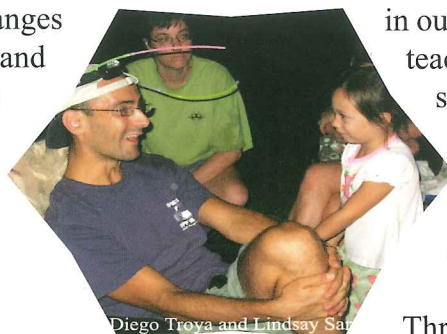


Go Yee!

For several years now, Prof. Gordon Yee has served the Chemistry Department in a very unique role. It's a bit tough to give a precise title to that role, but it ranges from being the conscience of the Department and its Chair (providing honest advice, alerting us when something isn't quite right, etc.) to being a tireless advocate for faculty and students (especially when it comes to awards and recognition) to organizing activities that have a positive effect on morale. In the latter context, Gordon has arranged a slew of activities including the now legendary "Iron Chef" competitions (pitting various groups of students/faculty against each other) to Chili cook-offs (where cash prizes are awarded in various categories). Last year Gordon made the observation that most of what we do tends to be centered on food and eating. The net effect was that Gordon's singular comment set the theme for several Chemistry Department activities in Fall 2010 that took full advantage of the scenic beauty of Blacksburg and its surroundings.

In August, chemistry faculty organized our first (in recent memory at least) departmental camping trip. To keep things simple (and reasonably local), the destination was set to be the Rocky Knob

campground, just beyond Floyd, Virginia on the Blue Ridge Parkway. Friday evening was lovely, both in terms of weather and the company. There was the traditional campfire, and plenty of food and drink. Of course, faculty in our department are great teachers, and Prof. Troya saw this as a great opportunity to teach the children how to make Greek letters out of light sticks.



Throughout the semester, Gordon has organized various hikes (inviting graduate and undergraduate students to join with the faculty) including the Cascades/Barney's wall, Kelly's Knob, and Angel's rest.



Even our newest faculty member, soon-to-be Prof. Amanda Morris got involved, enjoying a hike to the Cascades in February.

If you have the opportunity to visit your alma mater, be sure to take the opportunity to enjoy the scenic beauty and countless outdoor recreational activities that this area has to offer. Chances are... it won't be difficult to find someone in the department who will join you.

Awards



Timothy E. Long (Ph.D. '87), Macromolecules and Interfaces Institute and Department of Chemistry at Virginia Tech and Dr. Carl Willis, Research Fellow, Kraton Innovation Center, Kraton Polymers, LLC

are the winners of the American Chemical Society Division of Polymeric Materials: Science and Engineering's 2011 Award for Cooperative Research in Polymer Science and Engineering. This award was initiated in 1992 when it was endowed by a generous gift from the Eastman Kodak Company. The 2011 award is based on the productive and sustained interactions of almost ten years between Prof. Long and Dr. Willis. An award symposium to honor the 2011 winners was held at the recent national ACS meeting in Anaheim.

.....

Tim Long Wins the Mark Scholar Award. The award was established in 2006 and is sponsored by Elsevier, the publishers of the journal Polymer. The award is administered by the Polymer Chemistry Division. Consideration for the award is given to research accomplishments and contributions to the advancement of polymer science through teaching, basic or applied research, technical leadership and scientific writings (such as technical journals or patents).



Judy S. Riffle (Ph.D. '81) has received the university's 2011 Alumni Award for Excellence in Research which is presented annually to as many as two Virginia Tech faculty members who have made outstanding

research contributions. Each recipient is awarded \$2,000. Riffle, who joined the Department of Chemistry in 1988, was 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.

New Building Award Davidson Hall Phase 1

Joseph Hoeflein of University Planning, Design & Construction at Virginia Tech, announced the approval by the state for construction. Funding to complete the design and for construction will be available on July 1, 2011. Construction contracts are hoped to be approved by December 16, 2011. Construction is expected to take place between January 2012 and January 2014 with substantial completion by year end 2013.

Student News



KASEY BEERNINK

Kasey is a senior CHEM BS major and a member of the Corps of Cadets. (Kasey's older sister is a CHEM & Corps alum.) Kasey is 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

Jennifer is a senior CHEM BA major who also played on the women's soccer team. She earned a departmental academic award (\$100) last year. Jennifer has earned an ACC postgraduate scholarship (The Weaver-James-Corriگان 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 will receive \$5,000 to contribute to their 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 V. BLAKELY

Martha, a junior chemistry major and member of the VT Varsity Tennis



team, talks about her philosophy of giving to her community in public service announcement co-sponsored by ACC and the United Way.

YI LI

Yi, a graduate student in Prof. Richard Turner's polymer research group, has



won the graduate category of the Fall 2010 OIRED/Phi Beta Delta International Experiences Speech Contest. In her speech "On a Journey Defining Myself," Yi Li reflected on the roles of language and networking, and on the value of persistence and openness.



Faculty Spotlight

Professor Felicia Etzkorn

Research in the Etzkorn group has blossomed in recent years with new projects in Environmental Chemistry and Chemical Biology. Many students still choose to do synthetic organic chemistry, yet these new directions have led to collaborations and funding outside of the traditional the Bioorganic discipline of design, synthesis, and bioassay. Dr. Etzkorn has enjoyed teaching a wide variety of both graduate and undergraduate organic chemistry courses over the past ten years. She especially has enjoyed creating two special new courses: Green Chemistry for undergraduates, and Chemical Biology for graduate students. She is happy to see that Green Chemistry has continued to grow and become even more popular in the hands of Professor Tim Long. Chemical Biology remains a small, interactive seminar course in which students read, present, and discuss papers on both historical and current topics.

In 2006, Dr. Etzkorn's friend and collaborator, Dr. Terry Hrubec, a developmental biologist and Professor at the VA-MD College of Veterinary Medicine, discovered that her control mouse fetuses were showing neural tube defects (NTDs) at unprecedented rates. Neural tube defects are perhaps best known from the work of the March of Dimes—spina bifida is the worst form in which babies survive, while cleft palates are the mildest form of neural tube defects. Although there is concern about the current research on NTDs in mice, there is little concern for humans, because NTDs in humans have been declining over the past 10 years due to supplementation of grain with folic acid, vitamin B9. Dr. Hrubec and her team narrowed down the source of the increase to the tap water. At that point, she enlisted Dr. Etzkorn's expertise as a chemist to identify the agent that caused the increase. Since then, chemistry graduate students, Jenny Pryzbyla, and Spencer Ahrenholtz, and Veterinary Medicine graduate student, Vanessa Keller-Melin, have been using GC-MS and LC-MS to apprehend the suspect(s).

Dr. Etzkorn has received the majority of her funding from the NIH over the years for her research on cell cycle regulation by the enzyme, Pin1. Pin1 binds to proteins containing the sequence phosphoserine-proline, so most of our designed molecules mimic proline in some fashion. Two approaches have been taken towards understanding how Pin1 regulates cell division: 1) enzyme mechanism studies with deuterium labeled substrates, and C-13 labeled Pin1, and 2) design and synthesis of small molecules that bind Pin1. The research has identified several inhibitors of the Pin1 catalytic activity, and several non-active site ligands that bind to a peripheral site of Pin1 called the WW domain. It is hoped that this two-pronged approach to target Pin1 will lead to anti-cancer drug lead compounds.

The signature Etzkorn group asymmetric syntheses of proline mimics to target Pin1, led them to investigate the role of proline in the stability of collagen. Collagen is the most important structural protein in our bodies. Biomaterials resulting from this research may find application

(Continued on Page 8)

Faculty Spotlight ... *(Continued from Page 7)*

in treating arthritis, burns, wounds, and other tissue repair. This work was funded by the ACS-Petroleum Research Fund and the NSF in recent years. In a decided about face, mimics of proline were found to destabilize the collagen triple helix structure rather than stabilizing it. At first a disappointment, these results have led to interesting new directions toward understanding the role of the prolyl amide bond in the triple helix structure.

Dr. Etzkorn came to Virginia Tech in 2000 with her family of five: two teenagers, Richard and Virginia, then two-year old, Galen, and her husband Dr. Richard Moore. In celebration, the family went on a trip to Provence in France for two weeks in August of 2000. Since Virginia Tech starts the fall semester earlier than most universities, little did she know that she would be teaching her first class in graduate Advanced Organic A on the very day she returned to a house and a lab full of boxes, jet-lagged and exhausted, to Blacksburg! After sleeping most of the previous afternoon and evening, Galen sat up in the hotel bed at 3:00 am, looked out at a streetlamp, and said, "Look Mama, it's morning!"

The Etzkorn-Moore family enjoys the Appalachians, the New River, and the Blue Ridge Mountains immensely, hiking, biking, and canoeing are favorite activities. Both Virginia and Richard have grown up to enjoy career as a public TV and ducer and landscape computer stop-mo-husband, Dick, is gomery Regional Dr. Etzkorn has been and knit a fair bit of In the 2010 calendar born to members lab specialist, Onyi Michael, in January, Chen had a boy, David, in July, shortly after Grace's Ph.D. defense, and Ana Mercedes-Camacho had a boy in September. And so, they've found themselves answering the age-old question, "Is it something in the water?" with the reply, "If so, it's not detectable!" All three were born big, healthy, and strong, with no NTDs.



DeSimone wins 2011 Harrison Howe Award

Joseph M. DeSimone (Ph.D. '90), Chancellor's Eminent Professor of Chemistry at the University of North Carolina, Chapel Hill, and William R. Kenan Jr. Professor of Chemical Engineering at North Carolina State University, is the winner of the 2011 Harrison Howe Award. The award is presented annually

by the ACS Rochester Section in memory of one of its cofounders. DeSimone, who is also founder of Liquida Technologies, in Research Triangle Park N.C., will receive the award during a ceremony in Rochester, N.Y. DeSimone's group is focused on learning how to bring the precision, uniformity, and

mass production techniques associated with the fabrication of nanoscale features in the microelectronics industry to the nanomedicine field for the fabrication and delivery of vaccines and therapeutics for the treatment and prevention of diseases.

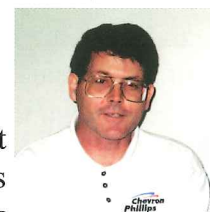
Entrepreneur

Frank Akers (B.S. '69), President-Techulon Inc., a life sciences company based in the Virginia Tech 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 around a beacon so scientist can follow its progress. "We're excited to bring this important technology to market,"

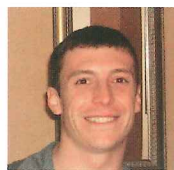
said Frank Akers, president at Techulon. "As treatments have become more targeted and cell-specific, clinicians need more integrated delivery and monitoring methods. Our goal with this technology is to deliver therapies to patients, and then image the precise location of the therapy and target," said Akers. "It is designed to help make treatments like cancer more targeted to tumor cell types."

Life Sooner

Be assured that everything is well with the Ed Boudreaux (B.S. '71) family and life with Chevron Phillips Chemical Company. We have been in Oklahoma long enough now (24 years), that we no longer lay claim to being East Coasters (although we still claim to be southern). In fact, we rarely get to the Virginia area these days. Our children and their families have established Oklahoma as their home state and it is likely that Linda and I will remain in Oklahoma upon retirement (which is not that far away). However, my years at Virginia Tech were formative and the memories are still good. In addition, the instruction I received has served me well both in my career and in life. So I still enjoy receiving news about the department.



Murphy appointed Assistant Professor



Dr. Brian Murphy (Ph.D. '07), was appointed Assistant Professor of Medicinal Chemistry at the University of Illinois, Chicago, in August 2010.

Ellison joins Bioformix LLC

Matt Ellison (PhD '95) has taken a new job at Bioformix LLC in Cincinnati, OH as Director of Adhesive Technology. The company develops new monomer material for coating and adhesive applications. Contact him at mattellison@bioformix.com.

(Continued on Page 14)

In Memorium



CHARLES 'CHUCK' GUSTAVUS HAAS, JR., 86, passed away of heart failure March 2010. Dr. Haas was born in Portsmouth, Va. He grew up in Portsmouth and Newport News and attended Virginia Polytechnic Institute, graduating with a B.S. in Chemistry in June 1944. Dr. Haas taught freshman chemistry and 400-level and graduate inorganic chemistry classes for most of his career at Penn State University. Dr. Haas retired from the university in December 1987.

Edward O. "Ed" Sternberg, age 88, of Knoxville, departed this life for Life Eternal on Nov. 15, 2010, as a result of lymphoma.

Robin D. Kinser, (B.S. '73), of Chesterfield, Va., died Wednesday, April 27, 2011, at home following a lengthy illness. She was born October 14, 1952, in Logan, W.Va., a daughter of Hazel M. Kinser of Mechanicsville, Va., formerly of Verdunville, W.Va., and the late Dallas A. Kinser. She was salutatorian of the 1969 class of Logan (W.Va.) High School, a National Merit Scholarship recipient, and was named a Presidential Scholar, representing the State of West Virginia her senior year; a 1973 graduate of Virginia Polytechnic Institute and State University, with a Bachelor of Science degree in Chemistry; a 1976 graduate of the University of Delaware with a Master's degree in Chemistry; and a 1993 graduate of the University of Delaware with a doctorate in Chemistry. She had achieved the position of Director of Analytical Research at Philip Morris in Richmond, VA., and retired from PM as a Senior Principal Scientist of Clinical Research after over 30 years of service. Ms. Kinser was an active member of the Women in Leadership and Philanthropy and the Chemistry Department Advisory Committee at Virginia Tech. She and her husband endowed the Dallas A. Kinser and Robert T. Johnson Memorial Scholarship in Chemistry at Tech. In addition to her mother, she is survived by her husband of 35 years, Michael T. Johnson; sister, Melody S. Kinser of Mechanicsville, Va.; and numerous more distant relatives. A memorial service will be announced at a later date. The Department of Chemistry will sorely miss Robin. She and her husband, Michael, have been major benefactors to the Department for many years.





Chemistry Faculty News



Karen Brewer: New Cancer Therapy appears promising in Pre-Clinical Trails. A new method for treating breast cancer is showing early promise in pre-clinical trials. The research team, led by Karen Brewer in chemistry and Brenda Winkel in biological sciences, along with Theralase Technologies, a manufacturer of medical laser devices, has developed a way to eradicate tumors without the harmful side effects of chemotherapy, radiation or a surgeon's scalpel. The group has built what Brewer calls a molecular machine: It seeks out fast-replicating cancer cells and becomes lethal only when exposed to light. When combined with a deep-penetrating laser from Theralase, the new molecule could help combat fast-growing cancers, such as breast, prostate, and lung, which up until now have not been able to be penetrated by light therapies.



David Kingston was appointed by Kathleen Sebelius, Secretary, U.S. Department 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 National Advisory Council is charged with the responsibility of advising, consulting with, and making recommendations to the Director, NCCAM, on matters relating to the research activities and functions of the Center. The role and responsibilities of the council members include secondary review of grant applications in light of NCCAM scientific program priorities and program balance.



Professor Louis A. Madsen has 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 Professor Martin Moller (synthesis – Aachen, Germany) and Dimitri Ivanov (structural and characterization – Mulhouse, France).



Professor James E. McGrath is 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 will use the \$100,000 award to investigate chlorine-resistant membranes for reverse and forward osmosis, nanofiltration, and waste water purification.



Professor Edward Valeev has received a four-year NSF grant (\$400,000) to work with collaborators at Stanford and Iowa State to develop sustainable software. Their objective is to enhance the accuracy of the software infrastructure for electronic structure theory. Their object 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.

(Continued on Page 12)

Chemistry Faculty News ... (Continued from Page 11)



Professor Harry C. Dorn's research program has been featured on Virginia Tech's home page. 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 radiotracing.



Prof. Judy S. Riffle has been 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 Robert B. Moore has been 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.



Professor Webster L. Santos and collaborator David Rekosh (University of Virginia) have 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.



Timothy E. Long, professor of chemistry in the College of Science at Virginia Tech, has been appointed the college's associate dean for strategic initiatives.



Master Teacher - Patricia Amateis

*Associate professor and director of general chemistry in the College of Science

*Coordinates more than 100 freshman chemistry labs

*Oversees more than 30 graduate teaching assistants as lab instructors

*Overall student-evaluation scores: 3.86 out of a possible 4.0

*Bachelor's degree in education from Concord College; Ph.D. (1984) in chemistry from Virginia Tech (L. Taylor-advisor)

Recognition

*William E. Wine Achievement Award, 2010

*Sporn Award for Excellence in Undergraduate Teaching, 1994

*Alumni Teaching Award, 2002

*Member of Virginia Tech Academy of Teaching Excellence

*Office of Residence Life Student Programs Division Favorite Faculty Award, 2006, 2007, and 2009

*Student Alumni Associates Students' Choice Award, 2004 and 2005

*Wrote comprehensive laboratory manual published by Hayden-McNeil

*Routinely speaks and gives chemistry demonstrations to schools and civic groups

Staff Spotlight

Roberta Gilbert

Business Manager for the College of Science,
Department of Chemistry

Roberta Gilbert started her career at Virginia Tech with part time positions in Architecture and Urban Studies, and business Affairs for Culinary Services before starting full time with the Controller's Office, and Continuing Education before joining The Materials Research Institute, The Center for Adhesive and Sealant Science, and the Department of Chemistry as support staff for the fiscal operations in April of 1998 and was promoted to the position of Business Manager in September of 2001.

Born in Wisconsin Roberta lived there until graduating from Reedsburg High School.

After traveling to Chicago summer as a nanny, she started a career Government by as Clerk for the Finance Center in She was promoted of increasing culminated her with the position with the office of the



*Roberta with daughter, Angie Kritak
(who also works in the department)*

Command, Foreign Military Sales for the Spanish Navy Ship Building and Modernization Program.

In 1990, Roberta and her husband, Jerry relocated their family to southwestern Virginia to be closer to her mother-in-law in her final years. The slower pace of the Virginia countryside was addictive and the family decided to stay. She proceeded to raise her two sons and one daughter in Giles County where she still resides. Her children have now married and are settling into Giles County. The family has grown to include six grandchildren. Some of her hobbies include reading, crocheting, and spending time with family and friends.

graduation, she to work during the Shortly afterwards, with the Federal obtaining a position Naval Regional Washington D.C. through positions responsibility and twenty-year career of Budget Analyst Naval Sea Systems

Expert Witness

James Rancourt (Ph.D. '87) In Polymer Solutions Incorporated's March 2011 newsletter (www.polymersolutions.com), founder and CEO, James Rancourt, describes what it's like to serve as an expert in lawsuits. He talks about the many different facets that go into serving as an expert. For instance, by agreeing to testify in court, there is often the implicit assumption that Rancourt will be available around the clock for the case, no matter what may be going on in his personal or professional life. Rancourt says his first case serving as an expert sticks in his mind. It involved involuntary manslaughter charges against a heating system repairman. The repairman stood accused of causing a home resident's death because the coroner's report indicated the presence of carbon monoxide in the deceased's lungs. The presence of the gas was taken as proof the man had died from carbon monoxide released by a heater incorrectly installed by the repairman.

The coroner used gas chromatography (GC) with a thermal conductivity detector (TCD) to determine the presence of carbon monoxide. It senses changes in the thermal conductivity of the gas coming out of the GC column and compares it to a reference gas. When an analyte emerges from the column, the thermal conductivity goes down, and the detector produces a signal.

But Rancourt testified in court, TCD is not able to identify a chemical's identity. The coroner should have used a second different chromatography column or should have used a spectrometric detector. Further, the coroner had indicated an approximate concentration of carbon monoxide but did not account for the fact that carbon monoxide is present in the earth's atmosphere. The formation of carbon monoxide within the lungs of the decedent, post mortem, was also not addressed by the coroner result. The heating system repairman was acquitted!

Married Postdoc

Mathew Shoulders (B.S. '04), was married in Madison WI in April. During his undergraduate studies, Matt did research on collagen in the Etzkorn labs. He received a prestigious Homeland Security Fellowship, and went on to receive many other honors. He received his PhD in 2009 from UW Madison for his work on collagen in Ron Raines group. He is currently a post-doctoral fellow at Scripps with Jeff Kelly.

On The Move

Carl Heltzel (Ph.D. '93) joined the chemistry department at Clemson in fall 2010 to take an active role in undergraduate education. Before coming to Clemson, Dr. Heltzel served as Chief Technical Officer for the National Institute for Home-town Security, and before that, he functioned as a consultant for Global Environmental Awareness Resources, and as Senior Chemist at Corporate Environmental Risk Insurance Agency. Dr. Heltzel has held faculty positions at Transylvania University, the University of York-National Science Education Center, the University of Hawaii, the University of Kentucky, and Chaminade University.

Webcast Speaker

Nicholas Snow (Ph.D. '92) is Professor and Director, Academic Industry Partnership, Department of Chemistry and Biochemistry, Seton Hall University. Nick regularly is a speaker in a live webcast sponsored by LC-GC North America Magazine. The title of his presentation scheduled for later this Spring is "Faster GC ... or Fastest?". One may register free for these webcast at <http://chromatographyonline.com/fastest>. Nick can also be seen most Fall Saturday afternoons in Lane Stadium watching the football Hokies.

Donors

Appreciation is extended to all alumni, friends, faculty and organizations that have contributed to the Department of Chemistry at Virginia Tech over the years. Your gifts make a difference and can be designated for general department needs or specific programs and scholarships. The following names are donors for the period July 1, 2010 - December 31, 2010.

GENERAL FUND

Alumni

Maria Arner
Robert Bass
Edwin Boudreaux
John Charkoudian
Ben Esquirel
M. Furness
Elizabeth Gross
Gene Hall
Mitchell Koppelman
Roy Lewis
Kathryn Lysko
Michael Macon
Kimberly Morgan
Teresa Schaefer
Catherine Schenck
Emilie Siochi
Victor Sower
Thomas Tachovsky
Joseph Thrasher
Michael Tydings
Steve Unger
Eddie Watts
John Waymack
Dean Webster
Phillip Young
Mark Zingelman
Joseph Zoeller

Faculty

David Kingston
Larry Taylor

Company

Aerojet
Cook Enterprises
Gen Corp Fdn

FRIENDS OF LARRY TAYLOR CHEMISTRY ENDOWMENT

Alumni

Robin Kinser
Mitchel Koppelman
Roger Ogden
William Starnes

Companies

Minerals Technologies

HAROLD MCNAIR FUND

Alumni

Dorothea Jeffery
Xiaowei Sun

Company

Novartis

FRIENDS OF CHEMISTRY SCHOLARSHIP ENDOWMENT

Alumni

Roger Wayne Ogden

JIMMY VIERS FUND

Friend

Don D. Lee

SURFACE VS. EMAIL

Those friends and alumni who prefer to receive Elements via Email, please send your address to:
ltaylor@vt.edu.

Create a Chemistry Scholarship or Endowment

A scholarship or endowment in your name or the name of a special loved you is a gift that will live forever. You can help our students to become tomorrow's leaders in industry, academia, and medicine. The Department of Chemistry offers scholarships to both undergraduate and graduate students based on academic potential, academic performance, and financial need. Endowments in support of faculty can help us recruit and retain outstanding professors. For more information on how to create a scholarship for a deserving chemistry student or any other endowment, please contact Jim Tanko, chair of the Chemistry Department at jtanko@vt.edu or 540-231-6687.

Pin1 Enzyme Transition State Analogue

Professor Etzkorn's Research Group:

Pin1 is a pSer/Thr-Pro peptidyl-prolyl isomerase enzyme that regulates proper cell division, thus it is of interest in the treatment of cancer, Alzheimer's disease, addiction, and several other diseases. Grace (Guoyan) Xu (Ph.D. May 2010) synthesized a number of inhibitors of Pin1 in an effort to understand the catalytic mechanism of the enzyme. One of her inhibitors, a "reduced amide," really a tertiary amine, had an IC_{50} value of 6.3 μM . A simplified analogue was crystallized in the active site of the enzyme, revealing that His157 is positioned to form a potential hydrogen-bond with the substrate prolyl nitrogen in the transition state. In conjunction with solvent and secondary kinetic isotope effects measured by Ashley Mullins, and Ana Y. Mercedes-Camacho (Ph.D. in Biochemistry anticipated May 2011), we propose a twisted-amide transition state for the Pin1 enzymatic mechanism.

