SPRING 2014

ELEMENTS

The Alumni Magazine of the Department of Chemistry at Virginia Tech

In this issue

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Tell us your story

Do you have an interesting story that might be featured in Elements? Do you know someone who should be featured? Or, would you simply like to say hello?

Contact the Department Chair, Prof. Jim Tanko (jtanko@vt.edu)

The Chair's Corner

J. M. Tanko, June 2014

Welcome to the Spring 2014 edition of *Elements*. Without question, the 2014 academic year has been very good, but also very challenging for the department on many levels. Fortunately, the continued hard work and support of our students, faculty, staff, and alumni has proven vital in helping us navigate the challenges. Thus, this issue of *Elements* will be a mix of good and not-so-good news.

Sadly, I must report that Prof. Jim McGrath died in May. Jim was the face of polymer chemistry at Virginia Tech and the chief architect of a program that achieved international recognition. (Please see page 10 to read more about Jim's illustrious career, before and at Virginia Tech.)

In the Fall 2013 issue, I reported that the Davidson renovation project was on schedule, and that the new section of the building would open in January. Shortly after penning those words, we learned that would not be the case. I will spare you the gory details, but suffice it to say that the good news is that the new Davidson Hall wing opened in June. In what can best be described as a game of dominoes, we are shuffling research lab assignments to consolidate groups; some faculty members who have had their labs over three different floors of Hahn South will soon enjoy contiguous lab space on one floor! We are also trying, to the greatest extent possible, to ensure that groups that have related research interests—and that can share equipment—are located in close proximity.

The design of the Davidson labs represents a new format for us in that they are now a shared, common space. That is to say, rather than assigning a two- or perhaps four-person lab to a faculty member for research (as is the case for Hahn South), the labs in Davidson accommodate 18 – 24 researchers, and this space is shared among several faculty members. The theory/computation group (Crawford, Troya, & Valeev) have already moved their groups into a specially-designed space on the first floor and are fully operational. The second floor of the building will house the more bio-oriented research groups of Profs. Etzkorn, Grove, Josan, and Santos—and these labs are also well on their way to being fully operational. The third floor will house Profs. Brewer, A. Morris, and Tanko—all of whom have research interests that involve electrochemistry and photochemistry.

The Chair's Corner...

As of this writing, only Prof. Morris has moved her lab (from Hahn Hall South). The others are currently located in the Corporate Research Center, and will be moving in this month. (Our lease ends on July 31!)

I described this move and reshuffling as a game of dominoes, but it is going amazingly well. Again, the hard work, support—and admittedly when things go awry, the patience of our students, faculty, and staff—are making it work. Did I mention that Sharelle Dillon, our stockroom manager, moved her operation from Hahn South to Davidson in about a week with only a minor disruption of services? Or the heroic efforts of our analytical services division (Geno Iannaccone, Bill Bebout, Mehdi Ashraf-Khorassani) in moving an NMR and two mass specs from the CRC to Hahn South? Or the efforts of Tom Wertalik (facilities) and Larry Jackson (electronics) in facilitating/coordinating all of this? Or, in addition to those I have already mentioned, the efforts of Tom Bell, EMillie Shephard, Anna Hawthorne, Joli Huyhn—who helped clear out historic Davidson of equipment, papers, etc.—on short notice? (Part of the Davidson delay was due to storage of combustibles in the old building, which prevented the issuance of an occupancy permit for the new building!)

Also, this past Spring, the Chemistry Department had its first formal external review since 1999. The external reviewers were top notch: Martin Head-Gordon (Berkeley), Ned Porter (Vanderbilt), Elsa Reichmanis (Georgia Tech), Alex Scheeline (Illinois), and Dave Tirrell (CalTech). This followed an internal review and report that was finalized in Fall 2013. The reviewers made a number of specific recommendation for improving the department in terms of "hiring policies and interdisciplinary programs, adequate and safe research space, the future of the polymer program, and the related issue of faculty demographics, as well as the quality and support of graduate students." Some of these recommendations are within our power, and are being addressed. Others will require the support of upper administration, and I look forward to working with them to see these recommendations implemented. The Department of Chemistry Advisory Council (DCAC), and well as our broader network of loyal alumni, will certainly play a role in helping us in this effort in the form of advocacy. I am very hopeful that with the appointment of our new president, Tim Sands, that the timing of this report and the climate on campus will work to our advantage.

In other news, the Spring DCAC meeting was held again to coincide with our Undergraduate Research Symposium/Poster Session—with DCAC members serving as judges (Tom Piccariello, Rob Shenton, and Bill Starnes). The first place prize for best poster was an iPad mini, and the winner was Benjamin Kolb (Amanda Morris).

Once again, the chemistry commencement ceremony was held in downtown Blacksburg at the Lyric Theater. Our commencement speaker was Prof. David Kingston. Da urged our graduates to "be thankful for those have helped you get where you are today," whether it was a parent, friend, fellow student, faculty member, or anyone who had a significant impact. (To facilitate actual follow-up among our stellar graduates, David passed out pre-stamped envelopes to each member of the Class of 2014.)

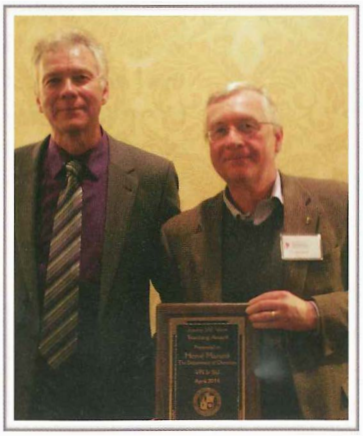
Finally, I want to close by mentioning members of our faculty and staff who were recognized this year for their accomplishments:

Joli Huyhn: Recipient of the 2014 Harold McNair Staff Service Award in recognition for her efforts as graduate student coordinator. Joli develops a rapport with our grad students before, during, and after they join the department. She arranges travel and lodging for their visits to campus during recruitment, interacts with faculty on graduate issues, and basically keeps the program running.

Amanda Morris: Recipient of the 2014 Alan F. Clifford Service Award in recognition of her efforts on behalf of the department and university. These efforts include graduate student recruiting, the chemistry Olympics (vide infra), her work as faculty advisor to oSTEM and Alpha Chi Sigma, and her general efforts related to diversity and VT's Principles of Community.

Webster Santos: Recipient of the 2014 John Sch Research Award, recognizing his work on sphingosine kinase inhibition, novel work developing catalysts based upon abundant (vs. rare and expensive) metals, and for his pioneering work on mixed hybrid diboranes. For those of you who frequent www.chem.vt.edu on a regular basis, you'll have noticed that Webster has been a staple in the news section this past year because of his research accomplishments.

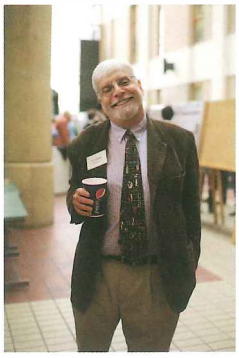
Herve' Marand: Recipient of the 2014 Jimmy Viers Teaching Award. Herve' has enjoyed success implementing the "flipped classroom model" in physical chemistry. This involves an online lecture, and in-class problem solving. He also is the instructor for the department's only online course (PChem for the Life Sciences), and earlier this year, offered this class as part of VT's inaugural Wintermester session. A student comment from one of these classes nicely summarizes Herve's approach: "Honestly, I think he did more w than the students!"



Life After Herding Chemistry Cats: *Perspectives From Our Former Chairs*

This is the first in a series of articles on how Chemistry's former chairs are spending their busy days

Prof. Joe Merola



When Jim Tanko asked me to describe life after being a department chair in a few words, I thought. "Heck, I can describe it in one – wonderful!" Now, don't get me wrong, being department chair for 6 years was probably the most rewarding time I have had here at Virginia Tech. Having the faculty, the staff and the students with which the department is blessed made representing chemistry a real joy. Being in a position to play a major role in the design of a new building was an opportunity of a lifetime.

Nonetheless, life post-chair has brought me back to the life I wanted when I left Exxon in 1987—a focus on teaching and research. Since moving from the department chair position, I now have a group of 6 graduate students and, over the past few years, anywhere from 3 to 10 undergraduates. The biggest part of "wonderful" is the time I now have to work on my scholarship. I have published 26 peer-reviewed papers in the last 3 years including a couple of papers in pharmaceutical journals. I am pleased to say that a patent has been allowed on a new class of anti-microbials (including compounds active against MRSA) and I hope we can continue development of these toward the ultimate of commercialization. I have also written quite a few grant proposals (please do not ask if any of them were funded – this is supposed to be an upbeat article.)

I have greatly enjoyed teaching our graduating B.S. seniors in the Inorganic Lab they must take – getting to know these fine young men and women as they embark on their chosen paths to graduate school, other professional schools, or into the workforce is a real joy that a department chair just does not have time for. This lab experience with our seniors also makes the Chemistry Department commencement ceremony all that more meaningful and enjoyable. In 2013, I won the Wine Award for Excellence in Teaching – one of the University's highest teaching awards.

For the 2013-2014 academic year, I was chosen to be the President of Faculty Senate at Virginia Tech, something that is not possible (or even allowed) when one is chair of a department. This position also gives me the privilege of being the faculty representative to Virginia Tech's governing board, the Board of Visitors. This year was an especially important year because this was the year of a search for a Dr. Steger's replacement; I was honored to contribute a small part in the selection of Dr. Timothy Sands as our new President of Virginia Tech.

I could go on and on to describe all of the things that are covered in the word "wonderful" but I suspect that Jim is not willing to let me have the entire issue of *Elements*. But, I do wish to say one last thing. Not being chair allows me to sit back and watch a superb department chair in action and know that the department is in fine hands. Thanks, Professor Tanko!

Prof. Richard Gandour

Jim Tanko asked me to describe life after being a department head, a position I took on in 1993. The department looked quite different then—Hahn South had just opened. Coming in as the boss and problem solver delayed my full integration into the Hokie Chemical Nation until 1998, when my term ended. I returned to my passions of discovering, mentoring, and learning. My proudest moments have been the graduations of doctoral students (Brett Kite, Winny Sugandhi, Richard Macri, André Williams, and Shauntrece Hardrict) and master's students (Jenny Kile, Sheng Tu, Marcelo Actis, and Brad Maisuria). My postdoctoral students (Yanyan Yang, Liang Chen, and Kyle Wilmsmeyer) have enriched my knowledge and served as mentors for the many undergraduates who have worked in my lab. Further, collaborating with my colleagues and mentoring their students has been richly rewarding.

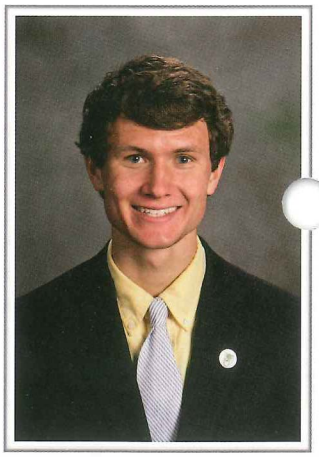
Getting back into the classroom to teach basic organic chemistry has been great fun. It has been both challenging and rewarding to develop new ways to engage a large class of today's students. An unexpected benefit has been the large number of undergraduate researchers who have joined our lab. In the last several years, we have had 15–20 undergraduate students working in the lab each academic term. Working with these young scientists has been rejuvenating.

As a final note, I have just spent the past year as Chair of the Departmental Review Committee, which chronicled the progress of the Department since 1999, the time of the last review. Compiling the data and assembling the document of the Department's growth and achievements these past 15 years has reminded me of how fortunate I am to work in such a great department. We continue to hire talented faculty members, attract promising students, and produce cutting-edge research. I look forward to the next decade of growth and achievements in the Department.

Keeping up with David Mackanic

Undergraduate Student Profile

Laurie S. Good



More often than not, a challenging class with an exacting instructor will deter a student from pursuing that subject as a major. Not so for David Mackanic of Cary, NC, a rising senior who is double majoring in mechanical engineering and chemistry. David initially had no intention of adding a chemistry degree to his academic pedigree, but his roommate (an ESM/biochem major) advised him to take Organic Chemistry during his sophomore year. He wasn't initially convinced that it was a wise choice for him—and actually remarked that the decision "was not well planned." Nonetheless, thanks to then-Chemistry instructor, Prof. Cindy Cribbs, who encouraged him to take the course and helped him prepare for it by giving him a "crash course review," he was hooked. In fact, David believes that "everybody should have to take Organic Chemistry. It provides a very different understanding of the world and explains a lot about *everything*." (Thank you, Prof. Cribbs!)

David Mackanic, a University Honors student, is among 283 sophomores/juniors from across the country awarded a prestigious Barry M. Goldwater Scholarship for the 2014-15 academic year. "Winning the Goldwater Scholarship is a great honor," David said. "I am very inspired by the research that I am involved in. The most meaningful aspect about the scholarship is that other people find my research compelling. It is great to explain why my field of research is important and have others agree."

Mackanic got involved in undergraduate research his first semester at Virginia Tech with a student outreach group called Bridges to Prosperity. They looked at concrete mixing compositions and techniques that may impact the strength of concrete used to build in third-world countries. He has also participated in two National Science Foundation funded Research Experience for Undergraduate programs. In summer 2012, David went to Beijing, China, to study hydrodynamic profiles of vibro-fluidized granular material. The following summer, he worked at MIT developing a method of creating new nanostructured materials that were highly effective as super capacitor electrodes.

Mackanic has worked on a variety of research projects with faculty at Virginia Tech, including the lab of Michael Ellis, associate professor of mechanical engineering, where he investigates novel materials for lithium air batteries. Robert Moore, professor of chemistry, jointly advises the project. "David is inquisitive, creative, and an extremely fast learner. When I explain things to students, I often start at an abstract level and then explain again with more detail or specific examples. The latter steps are rarely necessar with David as his insight allows him to quickly grasp new material. This characteristic is also apparent in David's ability to read technical literature, where I find that his depth of understanding is more appropriate to a second year graduate student than to a junior in his undergraduate studies," Ellis said.

Mackanic is also a member of the Honors Residential College, currently serving as a resident advisor. He is also active in the Intervarsity Christian Fellowship and the Ultrarunning Club at Virginia Tech, which has him participating in 7-8 marathon-length trail races a year. He'll have some interesting terrain to explore this summer once he joins Professor Graham Duncan at the University of Strathclyde in Glasgow, Scotland, in early June to conduct research on the synthesis of nanoparticles for energy harvesting.

After finishing his undergraduate degree, David will be pursing a Ph.D. in materials science—ideally at either Berkeley or Stanford—to develop novel materials for energy storage solutions. Ultimately, he would like to research technologies that can enable a society powered by renewable energy—mostly likely in industry where he eventually plans to start his own company. Once he does so, readers should buy stock early and often!

Giving Back: Taylor Mach

Graduate Student Profile

Laurie S. Good

With his 6.5 inches of thick, curly hair, soon to be Ph.D./MAED graduate Taylor Mach has the appearance of a supercool young chemistry professor. And given that his hair needs another two inches of growth before he can donate it to "Locks of Love," later this year, his VT summer session P-Chem students will no doubt breathe a collective sigh of relief when he walks into the classroom for the first time. But Taylor is remarkable for many other reasons.

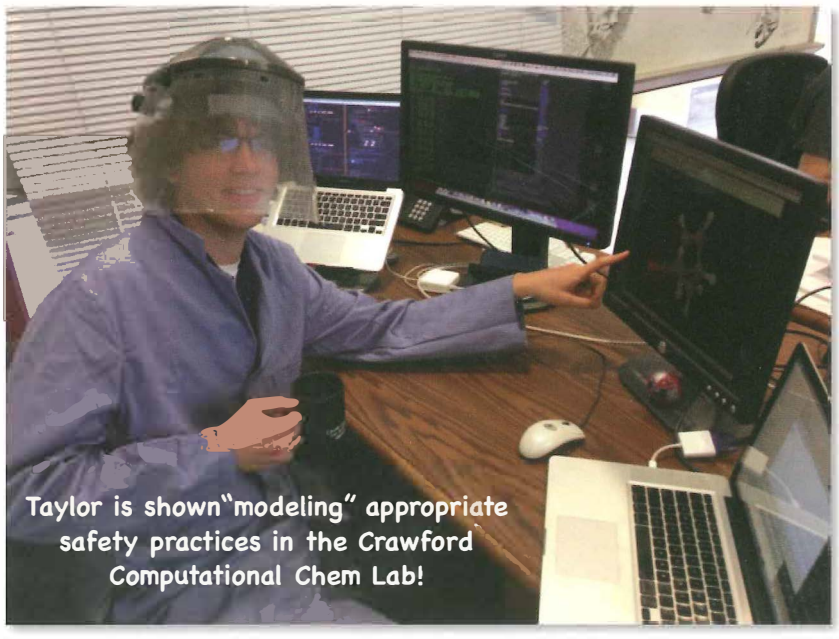
"Taylor once told me that he decided to pursue both a Ph.D. in chemistry and a master's degree in education as a way to "give back" after he had received so much himself from his teachers. To me that speaks volumes about his integrity and outlook."

Daniel Crawford, Professor of Chemistry

Born and raised in St. Paul, Minnesota, Taylor Mach is the son of a second grade teacher (Cindy) and a computer tech professional (Ron). Like many science majors, he became interested in chemistry as a possible college major as a result of a high school teacher who understood the value of a hands-on classroom experience. Even though Taylor (his high school's valedictorian) later entered Bethel University as an "undecided" major, it didn't take long for his academic advisor, Rollin King, a computational quantum chemist, to snag him. Because he missed general chemistry during his freshman year, Taylor studied the basics on his own over the summer and passed the ACS Gen Chem exam. Prof. King had another important connection in terms of Taylor's graduate school plans—he happened to have earned his doctorate from the University of Georgia alongside Prof. Daniel Crawford, Taylor's Ph.D. advisor. As a result, Taylor spent his junior year summer with Prof. Crawford, who offered him a research assistantship on the spot once he completed his B.S.

Since joining the Crawford group in 2009, Taylor's research has principally involved improving the quality of quantum chemical calculations of optical rotation. The requirements for predictive gas phase computation of optical rotation are well established, but the majority of experimental measurements are performed on solution phase samples. Taylor's most recent work has been developing and testing computational approaches that approximate solvated systems with the goal of creating a robust, cost-effective method that enables chemists to easily perform calculations of optical rotation. So far these tests have shown, as expected, that computing solution phase optical rotation is an extremely challenging problem.

While he enjoys the problem-solving aspect of his research, Taylor realized that he didn't want "the research lifestyle," which would likely involve more hours and be more solitary than he really wanted. Enter Virginia Tech's School of Education. Under the direction of Profs. George Glasson and Brenda Brand, Taylor will also be awarded his MAED (Secondary Science Education Master's). This semester he's been teaching chemistry in Roanoke County high schools in much the same way he first encountered chemistry—as a hands-on, engaging experience. For example, Taylor borrowed the infamous "potato cannon" from Prof. Gordon Yee to teach an AP section on gas laws. (No doubt at least one high schooler will decide to pursue a science major as a result of watching a spud traverse the length of a football field.) He also fixed the school's sole vacuum pump that had not functioned since 2002. Obviously, Taylor's become a pretty popular addition to the Roanoke school system.

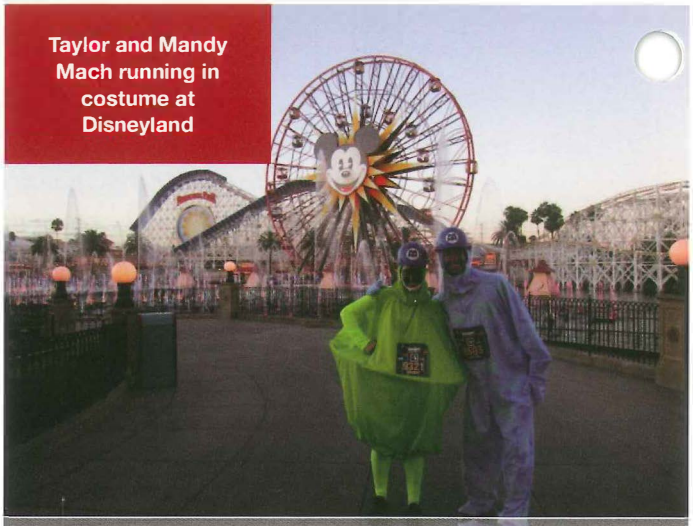


Taylor is shown "modeling" appropriate safety practices in the Crawford Computational Chem Lab!

Taylor Mach...

In the fall, Taylor will join Concordia University in St. Paul in a teaching position they created specifically to get him on board. When they learned of his dual degree they lobbied for funding to bring him to Concordia, which is known for teaching excellence and experiential research opportunities for its undergrads. The move back to his home town also suits his wife, Mandy Mach, who is a Blacksburg 5th grade teacher also earning her Master's in Education. They were high school sweethearts.

It the little bit of spare time he has to himself, Taylor is a skilled cook and *quasi*-avid runner. Mandy is probably the more dedicated runner of the two; in fact, she talked him into taking on "The Goofy Challenge" at Disney World in 2012, which according to their website is a "39.3 mile adventure held over two days; participants run the half marathon on Saturday, followed by the full marathon on Sunday." Finishing the Goofy Challenge earns the exhausted runner three finisher medals (Goofy, Donald, and Mickey)—not to mention the incredulous reactions of non-runners (the writer included!).



Taylor and Mandy Mach running in costume at Disneyland

Goofy Challenge Triple Medal Winners: Taylor and Mandy Mach

When asked about his overall experience at VT, Taylor replied that when he first considered graduate school, his goal was to make a significant contribution to the computational chemistry literature. And while he has certainly left a legacy for himself both here and elsewhere (Taylor presented his work in Switzerland, Denmark, and Spain while a graduate student with Prof. Crawford), he is far more satisfied with the lifestyle balance he knows he'll have at a smaller teaching institution...and with plenty of family members in the vicinity to help him shovel snow.

Davidson Hall Rededication:

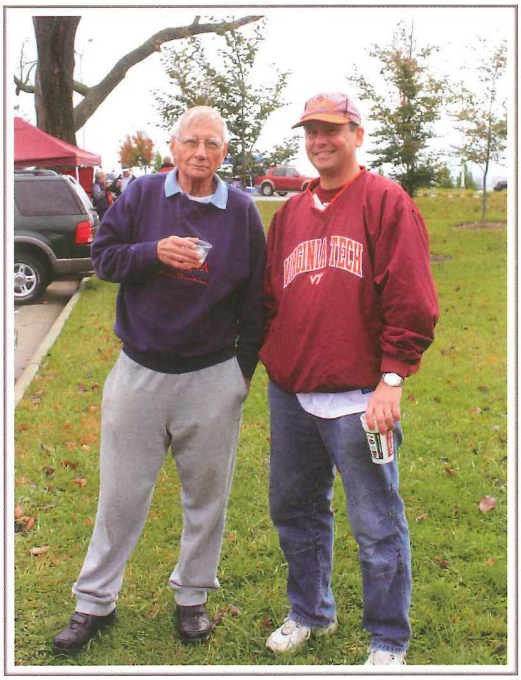
The Department of Chemistry Advisory Council (DCAC) is planning a "rededication" and alumni reunion ceremony to coincide with the completion of the renovation of Davidson Hall. We are conducting a survey to assess interest in this event and to get suggestions about possible activities. To participate, please go to:

http://goo.gl/XbXrdx

Chemistry, Hokie Football, and 25 Years in Academe

Alumni Profile: Nick Snow

I am honored to have the opportunity to share a bit of life during and since Virginia Tech, now more than 20 years after receiving my Ph.D. under the direction of Prof. Harold McNair. Today, I am Professor and Chair of Chemistry and Biochemistry at Seton Hall University. I started at Virginia Tech in 1987, the same year as Coach Frank Beamer, fresh from undergraduate school at that other large state institution about 150 miles north and east of Blacksburg. At that time, Coach Beamer was paid about 20 times the amount of a graduate teaching assistant; today, that differential has ballooned to about 100 times. I met my wife Angela (VT Biochemistry BS, 1990; and UVA PhD, Chemistry, 1995) at VT in 1989 and was easily converted to VT football.



In 1990 I had one of those nervous graduate student moments when I asked for permission from Prof. McNair to miss group meeting on a Saturday to attend one of the biggest football games in ACC history: 8-0 and consensus #1 UVA versus 8-0 Georgia Tech. UVA lost that game 41-38 in a classic matchup, starting a three-game slide capped off by a 38-13 loss to VT in Blacksburg. (Thank you, Professor Taylor, for getting us tickets to the sold-out final game!) As an aside, UVA received a Sugar Bowl bid just prior to that skid. The ensuing uproar led to formation of the Bowl Alliance, which led to the BCS, and ultimately to the upcoming playoff.

I completed my degree in 1992 and joined Angela in Charlottesville. I took a position doing GC-MS analysis in the drug testing facility at UVA, followed by a faculty appointment as Lecturer in Chemistry. I guess I had to leave to see VT become good at football and go to a bowl game. We traveled with the Hokie Club to the Independence Bowl. Flying into Shreveport, everyone was looking out the right side of the plane and cheering as we passed over the stadium and saw the VT logo in the end zone. At the next year's bowl game, a kid named Peyton Manning torched the Hokies, but it was a fun trip anyway.

Thanks to networking through L.J. Cline Love at SHU and Jim Demas at UVA (never underestimate the power of your professional network), I was encouraged to apply for an open position at Seton Hall in 1994. I was appointed assistant professor in 1994 and have been at SHU since. By 1995, Angela had finished grad school, ending a year of long-distance commuting, and we bought our first house in Rockaway, NJ. She started what has become a 19-year (so far) career as a Teacher of Science at Memorial High School in Elmwood Park, NJ. At the 1996 Sugar Bowl, Texas was dominating until Bevo the mascot (a very large longhorn bull) left a puddle on the Superdome carpet, VT intercepts; final score VT 28 Texas 10.

VT in the Big East was a special pleasure. I spent numerous afternoons and some evenings at VT-SHU sporting events. I was tenured in September 1999—the same fall as that magical Michael Vick-led run to the national championship game. We attended several games that fall, including Vick's 85-yard run at BC (with Greg Slack), the "miracle in Morgantown" run that saved the

Above: Nick Snow and Professor Harold McNair before a football game in Blacksburg, fall, 2010

Right: Dr. Angela Snow and Coach Frank Beamer at the Orange Bowl, 2011

...Nick Snow

the unbeaten season and the big game against FSU. Away games in the Big East were much easier to attend from New Jersey than home games. A surprise meet-up with the Taylors highlighted a trip to Syracuse in 2000.

At work I was serving as Associate Chair of the department and running my research group, doing all the usual things that academics do—teaching, publishing, attending conferences and chasing funding. I have been blessed with some once-in-a-career assignments. In 2001, I was appointed Faculty Chair of SHU's university-wide reaccreditation with the Middle States Association, which was completed in 2004. Regional accreditation is typically an every-10-year process that allows universities to demonstrate the quality needed to receive federal student aid funding.

In 2001, we moved to our current home in a wooded area in Sparta, NJ, with 4 ½ acres of mostly trees—somewhat reminiscent of Professor McNair's old place on the hill near Blacksburg. In 2003, I was promoted to full professor and became department chair. My Middle States work concluded with reaffirmation of accreditation and VT joined the ACC. We upgraded our Hokie Club membership and purchased season tickets. It's only a 500-mile drive. 2004-2007 saw SHU rebuilding the science building, with three departments still using it. For the many who have experienced the Davidson Hall reconstruction...I feel your pain, but it is well worth it.

Recently, I have been honored to experience senior administration as Associate Provost for Finance and Administration, responsible for SHU's $130-million academic affairs budget. Directly reporting to the Provost gave me a view of higher education that most faculty do not see. I encourage my academic colleagues to consider leadership at some point in your career. I'm now back in Chemistry and Biochemistry, teaching, mentoring students, writing and getting into the lab. Angela had 100% of her students score 3 or better on the AP Chemistry exam last year. Our most recent bowl game trip was the 2011 Orange Bowl. Yet another kid QB spoiled Tech's night: Andrew Luck who later replaced that other kid in the NFL.

I cannot be a prouder VT alumnus. As the football team rose to national prominence, so have the Department of Chemistry and the institution. **LET'S GO! HOKIES!**

Other Chemistry Alums News!

Dr. Abhishek Roy (MACRO Ph.D., 2008, Advisor J.E. McGrath) received the 2014 College of Science Outstanding Recent Alumnus Award, which is sponsored by VT's Alumni Association and given to a single individual from each college. Dr. Roy, the DOW Senior Research Scientist credited as the primary inventor of DOW FILMTEC™ ECO Reverse Osmosis Elements, has been named a recipient of Dow's prestigious Sustainability Innovator Award. With large-scale, positive sustainability impact, this technology was recently announced as Dow's second Breakthrough to World Challenges. The solution fights water scarcity by delivering 40 percent better purification with 30 percent less energy and has the potential to impact millions of lives. The technology has been commercialized into several different novel product offerings over the last 3 years. He also contributed in developing for the first time a novel 2D high temperature liquid chromatography separation method with applications towards fundamental and product development research for poly olefins, elastomer and other industrial polymers. The technology is patented and currently considered by third party for market introduction as a commercially available separation science characterization method.

Ms. Andrea Carlini (B.S. 2012) was recently awarded an NSF Graduate Research Fellowship for her work on "heart tissue repair with IV-injectable enzyme-activated biocompatible peptide hydrogels." Andrea is currently in the biochemistry doctoral program at the University of California San Diego. Her work on this project could help establish a new paradigm for the treatment of myocardial infarction, namely the use of IV injectable materials capable of initiating positive remodeling and healing immediately following heart attack, which is currently not possible.

Jeff Kerns (B.S. 1989) is currently employed at GlaxoSmithKline in the Stress and Repair Discovery Performance Unit (DPU) where he manages a medicinal chemistry group focusing on targeting therapeutics toward cellular stress and repair mechanisms.

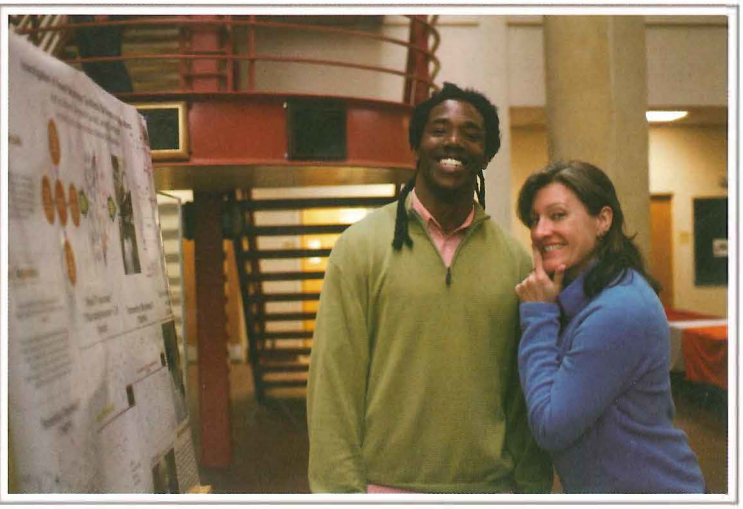
After over 20 years at Air Products and Chemicals, Inc., **Dr. Carrington D. Smith** (Ph.D., 1991, Advisor: Prof. J.E. McGrath) joined MPD Chemicals in February 2014 as their new CEO. MPD Chemicals is a US-based manufacturer of specialty chemicals with expertise in multiple technical areas including complex organic synthesis, unique monomers, polymer development, organosilicon chemistries and stable isotope labeling.

Dr. Yanpeng Hou (PhD, 2009), an Associate Principal Scientist at PepsiCo in New Haven, CT, was twice recognized as a co-recipient of a PepsiCo Pursue Great Science Visionary Award. One of the awards was for a natural sweetener project, and the second was for establishing a non-targeted metabolomics platform for product development and natural ingredient discovery.

Dr. **J. Paige Buchanan**, associate professor in the Department of Chemistry and Biochemistry at the University of Southern Mississippi, has been named *Chemist of the Year* by the Mississippi Section of the American Chemical Society. Buchanan has been at Southern Miss since 2006 where she teaches and maintains an active research group. She earned her Ph.D. in 1998 in physical organic chemistry under the direction of Prof. Jim Tanko, where she developed expertise in probing reaction mechanisms using a variety of techniques. She continued at Virginia Tech in a post-doctoral position in polymer science and joined a high-tech, small business entity specializing in advanced materials development for military applications. Buchanan has eight issued patents, authored 38 refereed publications and is author or coauthor of over 100 presentations at local, national, and international forums. In addition to her duties at USM, Buchanan is also an entrepreneur. In June 2008 she co-founded SciGenesis, LLC, a university start-up MURA company, with $2 million in funding to develop novel cosmetics and textiles for military applications.

Please keep in touch! If you have news to share for an upcoming issue of Elements, email our editor, Laurie Good, at lauriegd@vt.edu. We'd love to hear from you!

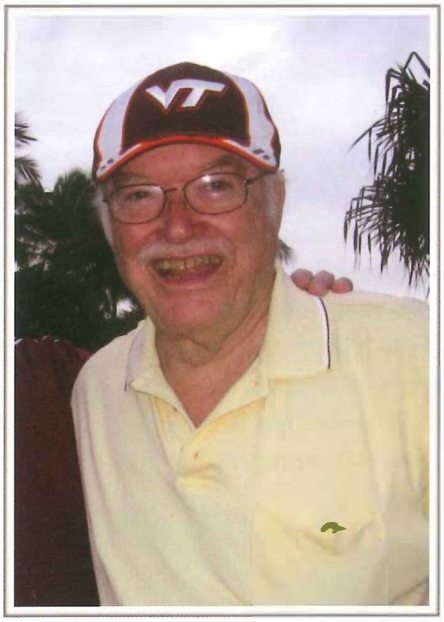
Student Poster Session, Department of Chemistry Advisory Council Meeting, Spring 2014 (Left: Recent BS Grad Steven Crane with Bill Starnes and Tom Piccariello; Right: Recent BS Grad Josh Moore with Dr. Maggie Bump)



In Memory: Prof. James E. McGrath

1934 — 2014

James E. McGrath, world-renowned polymer scientist and University Distinguished Professor at Virginia Tech died on May 18, 2014 in Blacksburg. Professor McGrath grew up on a farm in upstate New York and received his B.S. in Chemistry from Siena College (Loudonville, NY) in 1956. Jim used to say that one of the main reasons for becoming a chemist was so he could work indoors rather than face those hard NY state winters!



Jim obtained his master's degree in 1964 and his PhD in 1967 in polymer science working under Dr. Maurice Morton at the University of Akron. Prior to graduate school he worked on cellulose fibers at Rayonier, Inc. and then he worked at Goodyear Tire and Rubber Company during the first few years of his graduate studies. He joined Union Carbide Corporation after he received this PhD and worked in research in various areas of engineering thermoplastics and polyolefins. He moved to the Department of Chemistry at Virginia Tech in 1975 when polymer chemistry was accepted in the USA at only a handful of academic institutions. Jim was the principal architect of what became one of the leading programs in polymer science and engineering in the world. He was the leader of one of the first National Science Foundation's Science and Technology Centers (the flagship center program of NSF), "High Performance Polymeric Adhesives and Composites," from 1989 to 2000. He established a series of widely heralded ACS short courses in polymer science and polymer chemistry at Virginia Tech which remain popular today with over 6000 alumni from around the world. His collaborative research with Professor Garth Wilkes in the Virginia Tech Department of Chemical Engineering led to the Polymeric and Materials and Interfaces Laboratory which is the predecessor of the current Macromolecules and Interfaces Institute at Virginia Tech. Jim supervised over 100 Ph.D. students and more than 80 postdoctoral associates. Jim McGrath alums populate many leading university and industrial research laboratories around the world.

Jim recognized the importance of interdisciplinary research on complex and challenging problems in polymer science (years before this became an accepted academic endeavor), and his students carried with them Jim's great enthusiasm for interdisciplinary research. Jim received many awards and honors and among these were: election to the National Academy of Engineering (1994), election to ACS Fellow (inaugural class 2009), ACS Award in Applied Polymer Science (2002), ACS Award in Polymer Chemistry (2007) and the Charles G. Overberger International Prize for Excellence in Polymer Research in 2013. He shared the Paul J. Flory Award in Polymer Education with his Virginia Tech colleagues Tom Ward and Garth Wilkes in 2004 and was a member of the Society of Plastics Engineers Hall of Fame.

Jim McGrath was truly one of the giants in our field. His pioneering research resulted in more than 400 publications and over 40 patents. His coauthored book "Block Copolymers: Overview and Critical Survey" had significant impact in this important field. His broad based research ranged from new high temperature polymers for adhesives and composites to creative multiphase polymeric systems, novel ionic polymerization systems and fundamental mechanistic understanding in cyclic siloxane polymerizations and important new materials based on this chemistry. Most recently his research has focused on high performance polymeric membranes for fuel cells, water purification, and gas separations. He was in great demand as an industrial consultant and was a familiar visitor in the halls of many industrial polymer research organizations. His composite discoveries fly on many of our commercial jet aircraft and his wide-ranging papers are widely and often referenced. Jim dedicated much time to professional activities serving the ACS Division of Polymer Chemistry (POLY) loyally in every office. He pioneered the enormously successful POLY External Workshops and continued to chair various workshops through 2013. Jim McGrath was a wonderful friend for many in the polymer community. Jim's infectious smile, his fun-loving participation in meetings around the world, where he often was seen wearing his Virginia Tech cap while playing the trombone or piano, and his stimulating lectures on advances from his research group will be greatly missed.

Improvements to the General Chemistry Program: Lectures and Laboratory

Patricia Amateis, Director of General Chemistry

The faculty who teach in the General Chemistry program are always looking for ways to help the 2,000 students who take this class each semester succeed. To that end, we have made some changes to the General Chemistry classes.

It's no secret that many of our students are woefully under-prepared for General Chemistry—mostly due to weak math skills. For the first time, freshmen entering in August 2013 took an on-line Chemistry Readiness Test, which consisted of 20 math questions. Students with low scores were encouraged to take a Calculations in Chemistry course in the summer prior to the Fall semester (or during the Fall semester), thus delaying enrollment in General Chemistry until they were better prepared. About 100 students did so; data is currently being analyzed to determine the success of the prep course in preparing students for General Chemistry.

In the Fall 2013 semester, we began using an interactive student response system, known as iClicker, in our General Chemistry classes. With this system, the instructor asks a question (usually multiple choice) about the material just presented in class and students answer the question with a remote response device. Answers are collected by the instructor's iClicker base and the results of the poll can be displayed to the class. The purpose of the iClicker is three-fold: (1) class attendance is encouraged since students must be present to earn the points awarded for responding to the question and for answering correctly; (2) the iClicker encourages active learning; and (3) the instructor can quickly determine if students seem to have grasped the concepts presented based on the percentage of students correctly answering the questions.

We have been utilizing an on-line homework system in General Chemistry for several semesters, which allows us to assign graded homework without the burden of hand-grading hundreds of student papers! This past academic year we introduced two types of homework assignments: assignments with predominantly calculation problems, and assignments that helped students with the concepts. This latter type of homework is called Learnsmart with Smartbook. Smartbook is an adaptive reading experience in which students read sections in the electronic textbook to answer questions on electronic "flash cards"; the system keeps track of what the student does/does not know. With this system, our students are more engaged with the course material than in the past.

We also just completed our third semester of common time tests. All students take the same test at the same time in the evenings, outside of class. This guarantees a consistent experience for all students regardless of instructor. The consistency among all sections of General Chemistry has meant that students can attend help sessions conducted by any instructor and we have coordinated help sessions so that students can attend them at a variety of times.

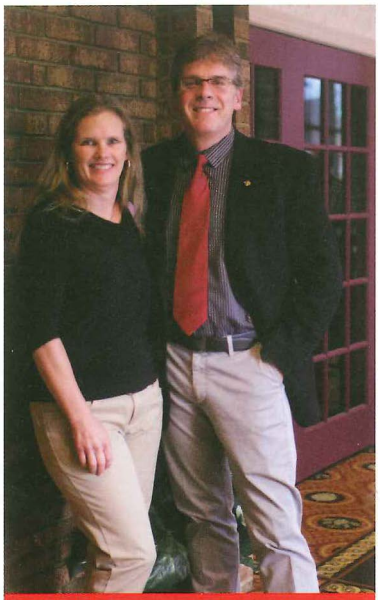
We still use recitations in the Spring semester (presented in a past edition of *Elements*). These small group (about 30 students) weekly recitations give students a chance to ask questions about the material presented in class, give them practice on problems (they complete a worksheet), and encourage them to study regularly since they are given a quiz each week in recitation. This past Spring 2014 semester, 27 junior and senior level undergraduates led a total of 54 recitations.

We are challenged by the number of students enrolled in General Chemistry lecture, by the diversity of preparedness of these students, and by the sometimes weak math skills of many of the students, but we continue to seek ways to give our students a solid foundation!

Victoria Long, Instructor, Polymer Lab/ Chemical Literation

"What is the function of the General Chemistry Laboratory?" Two different answers quickly come to mind: To provide a "hands-on" component to supplement the fundamentals and concepts concurrently taught in the general chemistry lecture, or to serve as an independent course with its own learning objectives and outcomes. Although the two are not mutually exclusive, beginning in Fall 2012 the two-semester General Chemistry 1045 and 1046 laboratory curriculum was designed to serve as an independent course.

The first semester laboratory course focuses primarily on teaching basic lab techniques and principles, understanding how to effectively use online resources and computers in the laboratory, and applying these foundations in real-life engaging experiments. Students learn accuracy and precision, learn common laboratory measurements techniques, learn about common laboratory glassware, and learn basic titration and weighing methods. Students learn to use excel for basic and statistical analysis, use word to format and display data tables with captions, use word to assist in technical writing, use Endnote to correctly cite literature references to avoid plagiarizing, and use Web of Science to find reliable literature references.



Vicki Long and husband Tim Long

The students complete two sets of round-robin experiments to investigate chemical reactions and processes, and complete real-life engaging experiments using state-of-art instrumentation rarely found in introductory general chemistry laboratories. The new experiments apply fundamental concepts and techniques to several real-life analyses used in research, commercial, and forensics laboratories. Students use Karl-Fischer titrators to measure the water content in commercial hand-sanitizer, use Atomic-Absorption (AA) to measure the iron content in Total cereal, use UV-Visible Spectroscopy to quantify the amount of cranberry juice in Cranberry-Apple juice, and use Gas-Chromatography Mass-Spectroscopy (GCMS) to determine if beach sand contains dangerous contaminants from a simulated chemical spill.

The second semester laboratory course builds on the foundation set in the first semester. Emphasis continues on using reliable Internet resources, referencing with Endnote, utilizing MS Office products effectively, and searching the literature for relevant current references. Experiments and laboratory questions often focus on applying the fundamental properties rather than simply measuring properties, i.e. how does the heat capacity of water influence cities located near large bodies of water? Students perform experiments focused on societally relevant topics including: Green Chemistry, Alternate Energy Sources and Water Investigations. Students synthesize and characterize the biofuel generated from the base catalyzed reaction of soybean oil, build a dye sensitized solar cell (DSSC), synthesize gold-nanoparticles (AuNPs) with tea leaves in an aqueous media, investigate protein folding and chemical bonding using Spirulina, and use GCMS to separa and identify chemicals found in common commercial pesticides.

The significant change in curriculum required changes within the lab protocol. Graduate teaching assistants (GTAs) now have more grading hours than in the past. Students submit more prelab and postlab assignments, which included six formal written reports each semester. To allow the GTAs additional time for grading and greater student assistance, a dedicated GTA provides twice-weekly help sessions and answers student questions using an online chat room. The online chat room has been very successful. Students post questions at any time of day in VT Scholar system. The GTA answers, or more correctly, guides the students to the answers. Therefore, questions and responses are available to all the general chemistry students, approximately, 2000 students each semester. Using the online chat room allows consistency among the answers, provides that all the students have access to th same responses, and allows the GTAs to als see and address students' questions. Additionally, several GTAs spend time in the Chemistry Learning Center (CLC) to provide assistance to students with their General Chemistry lecture courses. These GTAs assist with the online lecture homework, and provide tutoring prior to the exams.

Future plans include a greater focus on GTA training and assistance. The general chemistry laboratories cannot succeed without a strong GTA work force. Additionally, modifications to the curriculum will include adding several Problem Based Learning (PBL) experiments. PBL experiments allow students to define a problem and develop a strategy to solve or address the problem. While there has a been a significant change to the curriculum, one thing has not changed in 30 years; student evaluation comments often say "the laboratory course is too much work for 1 credit." There is no doubt that laboratory courses require significant time and effort!

There was Blood on the Court

Iris Carswell, former Chemistry staff member

This year's Chemistry Department Winter Olympics was certainly a violent one, with the eternal underdogs, the students, lashing out in desperation to win these high-stakes events. Prof. Amanda Morris tirelessly organizes these departmental competitions every two years to determine who is superior: faculty or student. While the answer may seem obvious (to some, at least), faculty members delight in watching their students try anyway.

This year's events consisted of basketball, laser tag, tennis, and skiing, taking place weekly throughout the month February. You may be thinking that these are not all technically winter sports—or hey, sports at all—but the funding did not come through in time for the bobsled track or figure skating outfits, so Prof. Morris had to make do.

First up was basketball. In a shocking turn of events, the students won – 18 to 6. It would seem that the faculty focused on careful strategizing too much, which turned out to be their downfall in the face of the wild and uncoordinated students' speed. The game ended as a smashing success for the students only halfway through when a bloodthirsty student viciously threw an elbow in Prof. Diego Troya's face. The faculty swore to take vengeance for their fallen colleague in the events ahead.

The following week was to feature a laser tag battle. Unfortunately, Mother Nature deemed this event unworthy of Olympic glory and proceeded to dump a few feet of snow on the East Coast to ensure it did not take place. Accordingly, the event was cancelled.

Next up was tennis. The snow had melted from the week prior and the matches took place on a gorgeous, shorts-worthy day. The two faculty teams consisted of Profs. Harold McNair & John Morris and Paul Deck & Gordon Yee, playing against the student teams of Emily Morris & Beth Childress and Eugene Camerino & Chris Houser. It rapidly became apparent that the students were just not up to snuff. The faculty routed them, winning every match easily and making it clear to the students that victory could be obtained without bloodshed.

The final event for these Olympics was skiing, held at Winterplace in West Virginia. It was Profs. Ed Valeev and Amanda Morris (supported by friend of the department, Kate Lucot) pitted against Ben Sundell, who alone carried the student team's hopes and dreams. The first head-to-head matchup was Valeev versus Sundell. The good professor was poised to win with a solid lead of about 15 feet. Upon realizing the devastation and humiliation the students would feel after being thoroughly annihilated in yet another Chemistry Olympics, he valiantly threw the match—figuratively and literally—by unselfishly flinging himself into the snow at the last turn. After a quick trouncing of Lucot by Morris, it was time to drive home to Sundell (and, by extension, all chemistry graduate students past, present, and future) the athletic superiority of Virginia Tech's Chemistry faculty. While it remains to be seen if that goal was truly achieved, Prof. Morris did succeed in winning versus Sundell by approximately half a ski length.

What good is a win without a little blood, sweat, and tears? No good, that's what. Bruised yet victorious, the faculty team has now swept both Chemistry Olympics held to date (not to mention an off-season softball event), thereby establishing both their intellectual and physical dominance over the students. The Chemistry Department Summer Olympics will be held in 2016.

Thank you for your continued support!

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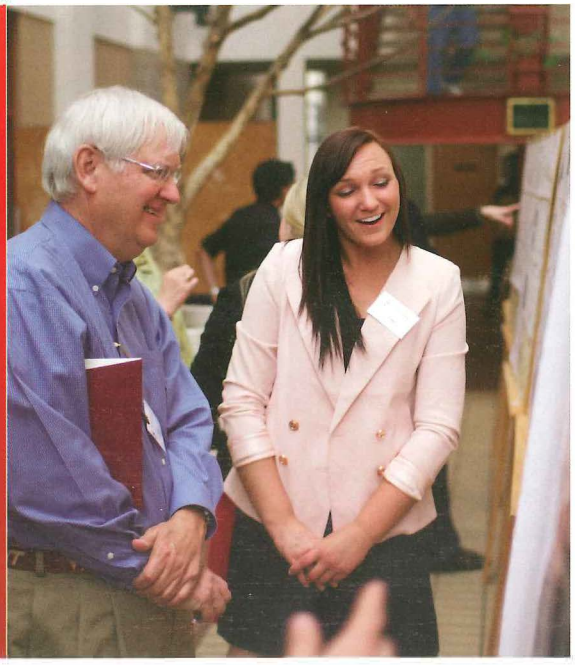
Donations to the Chemistry Department General Fund are used to support activities such as the Undergraduate Student Poster Session.



Giving Back

Support from alumni, corporate sponsors, and friends allows us to continue to invent the future

Every institution of higher learning is faced with increasing costs and diminished state funding. The Department of Chemistry at Virginia Tech benefits greatly from donations from its alumni, corporate sponsors, and friends in helping to bridge the funding gap. Unrestricted contributions to the department's general fund have an immediate impact on day-to-day operations. Working with its advisory council, the department has also established several endowed funds to address specific needs over the long term. Depending on their priorities and interests, donors may designate their gifts to one or more of these funds knowing that their gifts will go directly to that area of departmental need.

Donations to both the general fund and the endowed funds are needed and appreciated, helping the department in the short and long term. Contributions to the general fund are a primary source of discretionary funds at this time. Contributions to an endowed fund provide a steady, sustained stream of funding for the purpose supported by their fund.

The table below provides a brief rationale for each area, along with the information needed to direct donations to that area of need.

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We thank you for your support!

Name of Fund	Impact	ID Number
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This issue we feature the "energetic" contributions of Prof. Amanda Morris

Her current research focuses on two aspects of solar energy conversion: direct catalysis at photoactive electrodes and the development of solar cells from inexpensive materials. Ongoing efforts include: (1) Investigating the structure-function relationship of novel molecular materials for water oxidation and carbon dioxide reduction; (2) Utilizing pulsed laser techniques to investigate the photo-induced energy and electron transport; and (3) Exploring inorganic charge-transfer spin crossover complexes for use in low-cost, highly efficient quantum dot dye-sensitized solar cells.

Jim Tanko with Amanda Morris, this year's recipient of the Alfred F. Clifford Faculty Service Award