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#### **UPCOMING EVENTS**

Senior Awards Dinner May 4, 2010

Researchfest August 31, 2010

Procter & Gamble Lecture Prof. Paul Yager October 7, 2010

Stein-Bayer Lecture Prof. James Heath October 21, 2010



### UMass Amherst Chemistry– Energy Leaders

Energy is often called the "lifeblood" of our society. It keeps us warm, saves us time, gets us to work each day, powers our high-tech gadgets, and fuels the growth of our economy. As the global demand for energy continues to grow, there is a tremendous need to develop clean and renewable sources of energy to reduce our dependence on fossil fuels. To do this, significant advances in science and technology are necessary, and researchers in the Department of Chemistry are rising to meet this challenge. Indeed, through the work of two research centers on campus, which are directed or co-directed by Chemistry faculty, the Department of Chemistry is rapidly becoming a leader in energy research.

The two stories below give us an update about the Fueling the Future Center for Chemical Innovation and introduce the newly established Energy Frontier Research Center.

#### FUELING THE FUTURE



CCI group photo.

Phase I of the Fueling the Future Center for Chemical Innovation (CCI) was launched at the end of 2007 with funding from the

NSF Chemistry Division and specializes in materials chemistry for efficient charge transport in renewable energy applications. The Center is currently awaiting NSF action on its request to become a Phase II CCI, which would bring \$20 million of additional research funding to UMass Amherst over the next five years.

#### **ENERGY FRONTIER RESEARCH CENTER**

In April 2009, news came that the Department of Energy (DOE) had chosen UMass Amherst to host one of the new multi-million dollar Energy Frontier Research Centers (EFRC) to pursue basic research in



Prof. Paul Lahti

energy science. With a total DOE investment of \$16 million over five years, the UMass Amherst EFRC is poised to make major advances in the area of polymer-based solar energy harvesting and conversion. To find out more about this new energy center, we talked with Chemistry Prof. and EFRC Co-director Paul Lahti (PL).

### AN AWARD WINNING YEAR

2009 was a fantastic year for our faculty, staff, and students. Our faculty received numerous distinguished awards on- and off-campus. In fact, the Chemistry Department was the only department in the new College of Natural Sciences (CNS) to have faculty winners in all three categories of research, teaching, and service. With his Outstanding Service Award, **Professor Paul Lahti** is now the only individual to ever win awards in all three areas! Our staff and students also won important and well-deserved awards for their outstanding service and scholarship. The following is a list of our award winners.

#### **FACULTY**

Justin Fermann - 2009 CNS Outstanding Teaching Award

Jeanne Hardy - Lilly Teaching Fellow Award

Bret Jackson - Distinguished Faculty Lectureship

Paul Lahti - 2009 CNS Outstanding Service/Outreach Award

Michael Maroney - 2009 CNS Outstanding Research Award

Vincent Rotello - named fellow of the American Association for the Advancement of Science

Thai Thayumanavan - Samuel F. Conti Faculty Fellowship Award

#### **STAFF**

Marvin Ellin - 2009 CNS Dean's Service Award Victoria DeCarli - 2009 CNS Dean's Business Manager's Service Award

#### **STUDENTS**

Lawrence Borketey, Mariel Feliciano & Seena Koshy - CBI fellowship

John "Matt" Chudomel - Kuhn Graduate Fellowship

Kevin Early – Innovation Challenge Winner

Kevin Early - Richard and Meryl Brown Graduate Research Scholarship in Chemistry

Dan Fowler - Kuhn Graduate Fellowship

Ruthanne Hassey - Kuhn Graduate Fellowship

Bob Herbst - Kuhn Graduate Fellowship

Monique Johnson – Nano IGERT Fellow

Tejaswini Kale – Isenberg Scholar Award

James Kearns - Indo-US Science and Technology Forum (IUSSTF) / Oak Ridge Associated Universities (ORAU)

Research Internship in Science & Engineering (RISE)

Samantha Bernard Nicholls - Institute for Cellular Engineering IGERT Fellow

Matt Stevens - Residential First Year Academic Achievement Award

Elih Velazquez - Nano IGERT Fellow

## alumniNEWS

The following five alums have retired: **Jim Curley** (PhD '70) from Pfizer, **Al Blanchette** (PhD '71) from Personal Products Company, **Stephen Swarin** (PhD '72) from General Motors, **Ken Fletcher** (PhD '88) from The Foxboro Company, and **Gordon Cadwgen** (PhD '76) from DuPont.

Some current activities include **Mark Gelbert** (PhD '85) is Senior Vice President at Global R&D with Pfizer, **Joe Schlenoff** (PhD '87) is Chemistry Department head at Florida State University, **Dave Condit** (PhD) is doing fuel cell work at United Technologies in their Power Division. A student of **Prof. David Collard** (PhD '89) at the Georgia Institute of Technology has won the ACS Organic Syntheses Nelson J. Leonard Fellowship.

On a somber note, **Dr. Robert E. Graf** (PhD '72) died in November 2009. Over his career Bob worked at Varian Associates and IBM Instruments in high-pressure liquid chromatography. Later he specialized in computer applications and web development in the greater Washington, DC area. He helped develop the first web edition for USA Today, becoming its first webmaster. An obituary appeared in Chemical & Engineering News, Dec 14, 2009, p42. Also **Jim Driscoll** (BA '74) and **Larry Jaycox** (PhD '73) have passed away.

## alumni REUNION 2009

The 2009 Alumni Reunion was held on Saturday June 6 in the exciting new Integrated Sciences Building. Department Head, **Bret Jackson**, opened festivities with welcoming remarks. Twenty-nine people attended including 12 alumni, 5 staff and 12 faculty members. Attendees were thrilled with the new Integrated Sciences Building. Almost all of the entire 2nd floor atrium was used to display posters highlighting current academic/industry partnerships and to socialize and enjoy refreshments.





Visiting Prof. Ray D'Alonzo talked

about scientific pursuits in the industrial sector noting their high rate of failure and interestingly how that failure rate can be mitigated when academic collaboration is involved. The talk also included a walk down memory lane describing Ray's experiences at UMass Amherst as a graduate student and contrasting it to his recent experience in returning to academia after 31 years in industry. His talk was humorous and undoubtedly

helped the alumni present to relate. Ray's talk was preceded by Dean Jim Kurose's brief address about the many activities in the chemistry department and the new

buildings on campus.

Finally, special recognition goes to the following attending alums who celebrated reunion anniversaries of 50 or more years.

Allen Bluestein (BS '49), Danute Basiulis (BS '59), Juanita Bradspies (BS '59), Maureen (Casey) Hanlon (BS '59), Alphonse Plaza (BS '56, MA '59)



Professor Ray D'Alonzo

## metawampeAWARD 2009



The Metawampe Club is pleased to announce that it has awarded its first Metawampe Hike Award to Thomas F. Foley, a chemistry major from Longmeadow. This \$500 award, sponsored by an anonymous donor, is given to a chemistry major who is a member of the Club and exemplifies high academic achievement and professionalism in the chemistry department. The award was made at a brief ceremony Friday, December 4, 2009 by Prof. Ed Voigtman, Grand Sachem, and Prof. Dave Adams, Keeper of the Wampum. Tom is a 2008 graduate of Longmeadow (MA) High School in his sophomore year at UMass Amherst. He is presently collaborating with Prof. Justin Fermann in an analysis of the reasons for the ionization constant of hydrofluoric acid. Tom, a double major in chemistry and history, chose chemistry as his primary major due to the influence of his enthusiastic high school teacher. He participated in

the 2008 Chemistry Olympiad held here at UMass Amherst. The Metawampe Club, founded in 1907, hopes to continue to make this award if it has sufficient funds in its treasury.

# POINTS PRIDE in Chemistry

- Prof. Auerbach's images of zeolites featured on the cover of the *Journal of Physical Chemistry*.
- Prof. Dubin was awarded a grant for \$100,000 from the American Chemical Society for work on polymer-surfactant systems.
- Kevin Early (Prof. Barnes' group), one of the three members of QD Tech, won the UMass Amherst Innovation Challenge and received the \$35,000 grand prize for plan to improve solar cell output.
- Marv Ellin received a NSM Dean's Service Award for his many contributions to the college, particularly the planning, execution, and opening of the Integrated Sciences Building.
- Prof. Gierasch received the Dorothy Crowfoot Hodgkin Award from the Protein Society for her research in protein science.
- Integrated Sciences Building (ISB) was dedicated on Monday, Sept. 14, 2009.
- Tejaswini Kale (Prof. Thayumanavan's group) was a 2009-2010 recipient of the prestigious Isenberg Scholar Award created to encourage the integration of science and engineering with management.
- James Kearns (Prof. Tyson's group) was awarded a research internship in the Indo-US Science and Technology Forum (IUSSTF) and Oak Ridge Associated Universities (ORAU) Research Internship in Science & Engineering (RISE) program.
- Prof. Lahti, co-PI, selected for multi-million dollar Energy Frontier Research Center to advance energy alternatives and create jobs.
- Prof. Martin was awarded a \$45,000 special grant from the Camille and Henry Dreyfus Foundation to create a "Molecular Playground," a three-dimensional, interactive display of biologically significant molecules.
- Prof. Martin and graduate student Xiaoqing Liu discover how cells create stability during critical DNA-to-RNA transfers.
- Prof. Rotello and graduate student Bappaditya Samanta featured in *Science Daily* for creating an environment where magnetic particles suspended in solution help organize free-floating human cells to form chains and may be used to create human tissue.
- Prof. Rotello and colleagues design a "Chemical Nose" array of nanoparticles and polymers to sniff out cancer earlier and improve treatment options.

- Prof. Rotello was recognized for "distinguished contributions to supramolecular chemistry, particularly the use of nanoparticles in self-assembly and sensing."
- Prof. Tyson featured in the *Journal of Analytical Atomic Spectrometry* for developing the first accurate test for arsenic compounds in soil.
- Prof. Thayumanavan featured in the Royal Society of Chemistry for developing a three-component polymer that can respond to temperature, pH and the presence of a reducing agent.
- Prof. Thayumanavan's research on a new three-part polymer and its pharmaceutical applications featured in *Chemistry* World.

## labnotes

#### In the Auerbach lab ...

This has been a most exciting year for Prof. Scott Auerbach, his research group, and group alumni. Professor Auerbach won several new grants this year related to his work in biofuels in collaboration with Prof. Huber from Chemical Engineering. The new National Science Foundation grants are: "Modeling Shape-selective Base Catalysts for Making Biofuels," and "Energy Frontier Research Institute in Catalytic Pyrolysis of Biomass." Professor Auerbach also won a Department of Energy grant in "Energy Frontier Research Center on new Catalysts for Biofuels." In support of this research, Prof. Auerbach traveled to Brisbane, Australia to give a keynote lecture on "Modeling the Dynamics of Organic and Inorganic Networks," and to Bucaramanga, Colombia to give a series of lectures on "Theoretical Chemistry in the Design of New Materials for Renewable Energy Applications." Among the articles published by the Auerbach group this year, particularly exciting is an 18 page report in the Journal of the American Chemical Society on theory and NMR of new nitrogencontaining zeolites, which one referee suggested would "become the classic paper in the field." Professor Auerbach also led an exciting new educational project called "iCons" involving the development of new integrated science concentrations focusing on Renewable Energy, Biomedicine, Climate Change, and Clean Water. iCons has gained support from the highest levels at UMass Amherst; we hope to launch iCons in Spring 2011. Professor Auerbach is enjoying a well-deserved sabbatical at the University of California, Santa Barbara during January-June 2010, studying new fuel cell materials.

In group news, Karl Hammond defended his PhD in Chemical Engineering, and is now a postdoc in Nuclear Engineering at the University of California, Berkeley. Present members of the Auerbach group Vishal Agarwal, Julian Santander, Lin Jin and Dr. Ateeque Malani gave research presentations at the 2009 National Meeting of the American Institute of Chemical Engineers in Nashville, TN. Former members Ethan Sullivan, Leanna Toy, and Julia Kumpf are now high school chemistry teachers: Ethan in Southern California, Julia in Chelsea, MA, and Leanna in Amherst, soon to be teaching Prof. Auerbach's own children. Aldo Combariza finished his PhD in Valencia, Spain, and Prof. Cristian Blanco is now the Head of the Chemistry Department at the Universidad Industrial de Santander in Bucaramanga, Colombia. Professors Auerbach and Blanco shared many memorable moments during Prof. Auerbach's trip to Colombia, like the one shown below featuring matching sombreros.



Professors Blanco and Auerbach

#### In the Barnes lab ...

In the past year, Prof. Mike Barnes received new grant support from the NSF ("Single-molecule spectroscopy of Chiral Nanosystems") in collaboration with Prof. D. Venkataraman (\$420,000 in total costs through 2012). In addition, he was co-investigator and team leader on the newly funded US Department of Energy EFRC at UMass Amherst led by Tom Russell and Paul Lahti. Barnes continued work under the support from the US Department of Energy on "Chemical Microscopy of Conjugated Nanomaterials" for \$390,000 (through 2011), and became a member of the executive committee of the NSF-Center for Chemical Innovation (CCI: Fueling the Future), as well as continued participation in the NSF-Center for Hierarchical Manufacturing, and the Polymerbased MRSEC here at UMass Amherst. Professor Barnes also gave four invited lectures this year, served as Co-Chair for the Optical Society of America's Frontiers in Optics/Laser Science National Meeting in Fall 2009, and received a nomination for the Distinguished Teaching Award.

Our group members and research news: Ruthanne Hassey, Barnes' first graduate student, graduated from UMass Amherst with a PhD in Chemistry in August 2009. She is now a postdoctoral researcher with Prof. Bart Kahr at NYU in New York City. Michael Odoi, a 5th year graduate student, is now finishing up his PhD research on time-resolved spectroscopy on single molecules and nanostructured systems and will

be defending his thesis research this spring. **Kevin Early**, now a fifth-year graduate student, focuses on polarization properties of fluorescence from nanostructured materials, and his discovery of polarization-driven directionality in surface-derivatized quantum dot systems was published in ACS Nano earlier this year. **Kevin** also received the prestigious \$5000 *Richard and Meryl Brown Fellowship* for outstanding research in Chemistry in August 2009.

Austin Cypersmith is a new addition to the group and has been investigating single-molecule spectroscopy of chiral molecules in connection with our newly funded NSF program Yikuan Wang is a new postdoctoral associate in the group. He received his PhD in Physics from Marc Achermann's group at UMass in August 2009 and joined the Barnes group in October. Yikuan is working on several projects involving polarization and wavelength resolved measurements of charged-quantum dot systems and their application to local probes of charge-transport in thin-film optoelectronic devices.

A number of undergraduates have made significant contributions to our group's research efforts: **Joelle Labastide** (ChemE '09), **Joe Ryan** (BMB/Chem '09), **Joe Polak** (Chem '09), and **Artem Maksov** (Chem '09).

#### In the Chambers lab ...

The Chambers lab is booming. The lab is continuing to develop new drugs and chemistry-based tools to study some very basic functions that many take for granted. The "big picture" that the lab is trying to develop is an ultra-resolution understanding of how memories are formed in the human brain. The current state of technology is a bit like watching a soccer game on television through a foggy window. We can make out things moving on the screen, but we have no idea who the players are and no idea what they are doing. It is really just a blur. The technology the Chambers lab has developed will clarify this picture. After a marathon synthesis of the molecular core, initial testing shows that the new technology can mark individual brain synapses. This data, coupled with a new Alzheimer's Disease target and completely new therapeutic guarantee an interesting upcoming year.

The lab is still growing. There are now five Chemistry graduate students (Nate Akey, Mariel Feliciano, Jamie LaFrance, Amanda Hussey, and Steve McCarron), one Neuroscience and Behavior graduate student (Rosie Combs-Bachmann), and one Molecular and Cell Biology graduate student (Kathryne Medeiros). In addition, Vytla Devaiah continues to crank out synthetic molecules as a post-doctoral fellow and all the while has somehow found time to learn patch clamp electrophysiology and fluorescence imaging! Last but certainly not least, the lab has been a home-base in LGRT for no less than ten undergraduate students with majors ranging from Neuroscience to Biology to BMB to Chemistry throughout the year. The students make the cutting edge work possible and it

is absolutely wonderful to see so many young people excited about and involved with research at the neuroscience / biology / and chemistry interface.



Chambers group 2010

#### In the D'Alonzo lab ...

With respect to managing industrial collaborative projects, the second meeting of the Fueling the Future Center for Chemical Innovation Industrial Advisory Board (IAB) took place in October which provided useful feedback to the Center in terms of industrial requirements for fuel and photovoltaic cells. Discussions are now taking place with several IAB members regarding additional collaboration opportunities such as industrial research internships for graduate students working in the Center and potential contract research opportunities. Outside of the Center, discussions are in progress on micelle sensing technology with a major consumer goods company as well as discussions on the production of natural flavors using novel chemistry with an international flavor company.

In addition to industrial collaborative efforts, research has gotten under way in the last year in the D'Alonzo lab. Specifically, important synthetic work to prepare select mono- unsaturated lactones by undergraduates Melissa Gold and Kyle Bernier for use as mass spectrometry reference compounds is well under way. These non-commercially available reference compounds will facilitate the identification of new lactone flavor compounds in dairy products. Earlier careful capillary GC/MS/sniff-port aroma profiling work identified two new potent trace monounsaturated lactones of interest in butter. However, their electron ionization (EI) mass spectra lack sufficient information to determine their exact structural formulas. EI spectra from the synthesized reference compounds are hoped to facilitate the elucidation of their specific structures.

Progress has also been made at assessing the feasibility of performing liquid chromatography on the nano-scale. This challenging project involves the collaboration of several faculty members – Ray D'Alonzo, Matt Holden, and "Thai" Thayumanavan of Chemistry, Jonathan Rothstein of Mechanical and Industrial Engineering and Tom Chester of the University of Cincinnati. The goal is to demonstrate that two compounds can be separated in approximately 1 millisecond using parallel functionalized nanopores.

Theoretical work suggests that these pores should provide adequate resolution while only taking 0.2 seconds for well retained peaks to elute. Further, because of slip angle effects that occur on this scale, separations may be possible at reasonable pressures. Ideas for sample loading and ultra fast detection also appear feasible. Reducing the concept to practice over the coming year is the goal of the collaborating group.

#### In the Dubin lab ...

In 2009, Basak Kayitmazer (PhD '07) entered the faculty at Bogazici University (Chemistry), bringing to five the number of Dubin group alumni in faculty positions. Between setting up a new lab and teaching GenChem, she still managed to get a €100K Marie Curie EU grant, the first in her department. Emek Seyrek (PhD '05) was appointed lecturer at the University of Geneva also in 2009. Margarita Antonov (BA '09) saw her paper, co-authored with Malek Mazzawi (BA '10) appear in Biomacromolecules, and Elaine Foun (BS '10) co-authored a Langmuir paper based on collaborations with Matt Liberatore's group in Colorado. Other collaborations in stages of write-up, submission or publication in 2009 involved Denise Petri (Saó Paulo), Hervé Cottet (Montpelier), David Pink (Antigonish NS), and Julian McClements (UMass Amherst).



Prof. Dubin, Elaine Foun, Yisheng Xu, Margarita Antonov, Burcu Baykal, Kevin Chan, Ebru Kizilay

Ebru Kizilay began her research on polyelectrolye-micelle coacervates (a joint project with Tony Dinsmore, Physics) and Yisheng Xu made significant progress on stabilization and separation of proteins with polyelectrolytes, including the finding of selective binding with a polyelectrolyte to separate protein variants differing in only two amino acids. Burcu Baykal worked with Igor Kaltashov to develop SEC/MS methods to understand heparin-protein interactions. Ebru presented her work at a symposium on "Clusters" organized by Dinsmore and Dubin for a joint conference of ACS (Colloid Division) and IACIS; this and other presentations will appear in a special issue of Journal of Physical Chemistry to be edited by Dinsmore, Dubin and Greg Grason (PSE). Along with Basak Kayitmazer, Prof. Dubin organized a symposium on "coacervation" at the Fall ACS meeting, which will lead to a special issue in Advances in Colloid and Interface Science.

In addition to symposium participation and organization, Prof. Dubin gave presentations at Nestlé (Lausanne), Univ. Montpelier, Inst. Biol. Struct. (Grenoble), and more locally at Boston University, Genzyme, E Ink, and Pfizer.

Others joining the Dubin lab in 2009 were Simona Maccarone (postdoc, joint with Physics), Kaimin Chen (visiting scientist, on a joint project with Prof. Rotello), Dmitriy Federenko (U3), and Binqian Zheng (Amherst RHS).

#### In the Gierasch lab ...

The Gierasch lab was eventful during 2009: The lab was very productive, with five papers appearing. A highlight was an invited article by Molecular & Cellular Biology (MCB) graduate student **Rob Smock** and Lila, which reviewed the dynamic properties of signaling proteins. This paper was featured in the April 10th issue of the journal *Science* and was chosen to illustrate the cover (image at the right)!



Gierasch group members presented their research at several important conferences, including the Protein Society Meeting held in Boston, the "Proteins" Gordon Research Conference in Holderness, NH, and the FASEB Summer Research Conference on "Amyloid Fibril Formation and Protein Misfolding" held at Snowmass Village, CO. Lila co-organized with Ivet Bahar of the Univ. of Pittsburgh a Keystone Symposium on "Protein Dynamics, Allostery and Function" in June in Keystone, CO, and Rob Smock presented his work at this meeting. Lila was invited to several scientific meetings all over the country and abroad, and her presentations of the lab research this year included three lectures presented in Texas as a Welch Lecturer, a plenary lecture in Barcelona, Spain at the "Barcelona BioMed Conference on Peptide Engineering: Therapeutic Peptides", and another in Halle, Germany at the Bunsen Symposium on "Structure of Amyloid Fibrils and Mechanism of their Formation."

Two summer undergraduate researchers, Elizabeth Vinson from the University of Dallas, TX and a mentored ICE IGERT summer student, Iviana Torres from the University of Puerto Rico, shared our lab life during the summer and presented posters at the end of their stay at the Summer Undergraduate Research Conference (ICE/HHMI). We were also joined by Amherst Regional High School Junior Shiyuan Liu for internships in the spring and summer.

We are very proud of our undergraduate student **Dave Paquette** whose awards are getting almost too numerous to list. He received the Biochemistry & Molecular Biology Hayes

Award, which helped support his research during the summer, a highly competitive Hughes Medical Institute Summer Research Internships, a Junior Fellowship, and a Microcal Scholarship. He was invited to present his research as a talk in the undergraduate symposium at the Protein Society Meeting in Boston. Dave also completed a major cycling landmark, as he and Lila rolled smoothly through the COVAC Century on their bikes in September.

**Professor Pat O'Hara** from Amherst College visited the lab for her spring semester sabbatical. We all enjoyed her visit as she contributed with her experience to the lab academic activities.

We are thrilled as the lab incorporated new people: Anne Gershenson joined us in July as Research Associate Professor, bringing her experience and instrumentation for single molecule and fluorescence correlation spectroscopy experiments. We are very excited with this new capability of the lab as it opens many avenues for our research. We also recently welcomed Santosh Kumar who recently received his PhD from Manipal University in India and has joined our lab as a postdoctoral fellow. Kristine Pobre, a student from the MCB graduate program, chose our lab for her doctoral studies; among other projects, Kristine will work on a simulation that predicts the "fate" of a model protein inside *E. coli*.

We said goodbye to one graduate student and two postdoctoral fellows: Jenny Maki, successfully defended her PhD work on the mechanism by which the *E. coli* protein SecA recognizes signal sequences for protein export, and then joined the group of Alexei Degterev at Tufts University Medical School as a postdoctoral fellow. Postdoctoral fellow Qinghua Wang recently left our lab to take a position in the Center for Bioinformatics & Computational Biology at the University of Delaware, and postdoctoral fellow Harekrushna Sahoo has joined the lab of Petra Schwille at the Biotechnologisches Zentrum der TU Dresden. We wish Jenny, Qinghua and Hare all the best.

Lastly, we are happy to announce the arrival of two babies, new members of the Gierasch scientific family: **Qinghua Wang**'s daughter **Amanda**, born in Jan 2009, and **Eugenia Clerico**'s son, **Linus**, born in November 2009.

#### In the Hardy lab ...

It has been a very exciting year. **Witold Witkowski**'s work on the structure of the active site of caspase-7 was published as the cover story in the July issue of *Protein Science*. **Kristen Huber**'s development of a new method for expressing and purifying peptides was also published in *Protein Expression and Purification*. **Sravanti Vaidya** solved a very challenging new structure of caspase-6, a protein involved in the development of Huntinton's disease. Her work was recognized with the **Peter C. Uden** award, sponsored by *Procter and Gamble* 

during the 2009 ResearchFest. Samantha Bernard was married in October, becoming Samantha Bernard Nicholls. In December she also passed her ORP and advanced to PhD candidacy for her work developing a new reporter of cell death. Post-doctoral fellow Sumana Ghosh has successfully synthesized several novel peptides including stapled peptides and stabilized helices. Undergraduate researcher Lindsay Dawson, a senior undergraduate, is working to design a new protease sensor as she prepares to graduate and attend graduate school in chemistry. Professor Hardy was recognized for her excellence in teaching by the awarding of a 2009 Lilly Teaching Fellowship from the UMass Amherst Center for teaching. For her, a memorable teaching moment of the past year occurred when the UMass Amherst Marching Band Tuba section interrupted her 300-student section of general chemistry in the new ISB one Friday to serenade her with Happy Birthday.



Prof. Hardy's birthday surprise.

Hardy was also a guest on WGBY's program EcoExchange to discuss her work with the Fueling the Future Center for Chemical Innovation to develop protein-inspired proton exchange membranes for use in hydrogen fuel cells. During the program she drove a model car that **Prof. Justin Fermann** engineered to run on pure UMass Amherst water. The program originally aired on August 12th and has been rebroadcast numerous times since. Pictured on the EcoExchange set with **Marla Michael** are host **Sandy Thomas**, **Prof. George Huber** (Chemical Engineering), and Hardy (left to right).



Prof. Hardy on WGBY EcoExchange.

In 2009 three new students joined the Hardy lab as PhD students, Daniel Seeman, Elih Velazquez, and Muslim Yildiz. All three of them are off to a great start with new projects on allosteric regulation of proteins that are important in human diseases. Genevieve Abbruzzese, who had spent the

previous two years as a research fellow, started graduate school in the Molecular and Cellular Biology program this past fall, not long after her wedding last July. She was a co-author with Samantha Nicholls on a very popular poster at the annual symposium of the Protein Society. Two new Post-doctoral fellows joined the group during the past year. Dan Fowler, a 2010 graduate of UMass Amherst Chemistry is working jointly with Lynmarie Thompson on the proton exchange membrane project. Jun Chu, who graduated from Hunan University in China joined the lab to work with Hardy and Prof. Kim **Tremblay** of the Vet & Animal Science Department to develop a transgenic mouse that will fluorescently report on cell death that occurs as a result of developmental processes or side-effects of drugs. This work was made possible by a new grant from the Center of Excellence in Apoptosis Research. The Hardy group has grown substantially during the past year and is practicing posing, potentially for a Pharmacia advertisement, here.



The Hardy group, 2009

#### In the Jackson lab ...

The Jackson group continued its theoretical studies of gassurface reactions, with a focus this past year on elucidating the dynamics of methane dissociation on Ni and Pt catalysts. Two postdocs, Sven Nave and Ashwani Kumar Tiwari, demonstrated that the observed strong increase in the reaction probability with surface temperature originated in a variation of the activation energy with the motion of the metal lattice atoms. Some aspects of this work, described in a recent *Phys.* Rev. Letter, were highlighted in the Jan. 25, 2010 issue of Chemical & Engineering News. This work was also presented at several invited talks last year, including a conference on the Riviera, France and last summer's Dynamics at Surfaces Gordon Research Conference. Professor Jackson completed his seventh year as Department Head on 9/1/09 and happily rejoined the regular faculty, where he now teaches General Chemistry. Last December he gave a Distinguished Faculty Lecture, receiving the Chancellor's Medal for his research accomplishments.

#### In the Kaltashov lab ...

2009 was a very busy year in the Kaltashov laboratory, which included publication of four papers and several presentations at scientific meetings and conferences, including several invited presentations. Our group also spearheaded an effort to secure an \$800,000 grant from the National Science Foundation to purchase a new state-of-the art mass spectrometer for biomedical research, which is scheduled to arrive on campus

in the Spring of 2010. The group continued to expand both in size (as a result of five exceptional graduate students, Adriana Zeledon, Guanbo Wang, Yao Lu, Shunhai Wang and Jin-Yi Lim joining us in February 2009) and the scope of the research work (as a result of establishing new collaborations with colleagues at UCLA and USC). Two of the group members (Agya Frimpong and Virginie Sjoelund) successfully defended their PhD dissertations.

Wendell P. Griffith (PhD '05), who is now in the third year of his faculty appointment at the Department of Chemistry, University of Toledo (Toledo, OH) received his first large grant from the National Science Foundation through the Major Research Instrumentation Program. After several years at Schering-Plough Research Institute, Ben Mohimen (PhD '05) opened a new chapter in his career and moved to Vertex Pharmaceuticals (Cambridge, MA).

#### In the Lahti lab ...

The Lahti group had an outstanding year. Professor Lahti gave the very first lecture in the new Integrated Sciences Building (ISB) as that facility opened for business on January 26, 2009. The lecture was at 8 a.m. in the main lecture theatre to the Organic Chemistry II, Chem 262 course. Professor Lahti received an Outstanding Service Award from the new College of Natural Sciences in fall 2009, in part for work done to assist with moving into the ISB. Lahti is the co-principal investigator and co-director of the \$16M Energy Frontier Research Center "Polymeric Materials for Harvesting Solar Energy" (PHaSE), funded by the US Department of Energy Office of Basic Energy Sciences. The Center came online in August 2009. Lahti was a keynote speaker and conference international advisory committee member for the International Symposium on Novel Aromatic Compounds satellite meeting "Diradicals and Multiradicals: Theory and Experiment," at University of Namur in Belgium, during 26-28 June 2009. In November, Lahti was also invited to be the international speaker at the 3rd Russian-Japanese Workshop on Spin Chemistry on Awaji Island, Japan. Finally, in December 2009 Lahti completed a 2.5 year term as Undergraduate Program Director for the Chemistry Department.

In group news, Naoki Yoshioka was promoted to full Professor at Keio University, at a remarkably young age. Richard Walton reports that all is well for his family. Richard's work at Goulston is challenging and practical -- he says it was a proud thing for him to see some of his recent work through from envisioning to large scale production. Hidenori Murata is now doing research on lithium ion battery power for automobiles at Nissan. He reports that all is well for him, Miho, and little Riko. Patrick Taylor is now a postdoctoral research associate working jointly with Prof. Frank E. Karasz and Lahti. David Modarelli says all is well at University of Akron. Andrew Ichimura reports that all is well, including his work at San Francisco State. Chunping Xie, Technology & Business

Development Manager at Milliken Materials Technologies (Shanghai) Co., Ltd., says all is well. Pamela (Shields) Hill notes that she has been at Astra Zeneca for 7 years, now as a Scientist in the Infection Chemistry group. She has gotten a Master's degree and is now collaborating with scientists overseas for the company. She reports that husband Tom Hill is working at Flexcon doing polymer chemistry. Ken Marby has moved back to the eastern half of the USA, joining Merck in Rathway, NJ. May (Jitapa Sumranjit) sends greetings from Thailand, where she continues her work with the National Nanotechnology Center. Hemali Rathnayake completed at postdoctoral stint at UMass Amherst in the PSE department in 2009. She is now an Assistant Professor at Western Kentucky University in the Department of Chemistry. She, Chandana, and Bhanuk now have a house nearby. Nibedita Sanyal reports that she has recently moved to St. Louis with a job offer at Washington University Medical School. Lora (Michalak) Field reports that children Rebecca and Dylan are keeping her and husband Jay pretty busy up in "the Great White North" (her words). Safo Aboaku reports that all is well in his job at University of Mississippi. He and his wife, Kate, are happy (and presumably busy) with their work, and watching son Kofi (not so little now!!) and daughter Akosua grow. For anyone else with group news to share, please send it to Prof. Lahti, and it will be posted as we have time to do so. Thanks to everyone for their updates!

#### In the Maroney lab ...

The Maroney lab continues to pursue nickel biochemistry in several directions including, cellular nickel trafficking (NIH), nickel toxicology (NIH), the structure and function of nickeldependent superoxide dismutase (NSF), and hydrogenase (another nickel enzyme) reaction mechanism and applications to energy science with support from MassCREST. The research on nickel trafficking has taken the lab into uncharted waters with the realization that nickel recognition is a protein allosteric mechanism. This has led to the need to identify protein binding partners in order to understand trafficking mechanisms. News from the Maroney lab includes the announcement that Robert Herbst successfully defended his PhD dissertation entitled "Structure and Function in a Nickel Metallochaperone, HypA and Nickel Dependent Superoxide Dismutase," and departed for a postdoctoral position at Boston University. The lab also welcomed a new postdoctoral scientist,



The Maroney group, 2010.

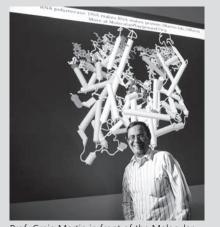
**Dr. Vlad Martin-Diaconescu**, who received his PhD for work done in **Pierre Kennepohl**'s lab at the University of British Columbia. Professor Maroney was elected Chair of the 2012 "Metals in Biology" Gordon Research Conference at the meeting in January 2009 and was recognized on campus with the 2009 College of Natural Sciences Outstanding Research Award.

#### In the Martin lab ...

Both current students and alums of the Martin lab continue to excel. Xiaoqing Liu successfully defended her PhD with some surprising results on the stability of transcription elongation complexes. In the field, we're used to representing a DNA duplex on paper as two parallel lines, but your average non-scientist will remind us that it is in fact a twisted helix. Xiaoqing's work, published in December in the Journal of Biological Chemistry, shows that it is the topological locking of the RNA "twisted" around the DNA that makes transcribing (elongation) complexes so very stable. Satamita Samata is now following up on this, attempting to show that an elongation complex with zero(!) base pairs can nevertheless be stable, stabilized only by the topological lock. On a completely different front, Ankit Vahia has solid results refuting a recently widely accepted model for abortive cycling in transcription initiation. While structures suggest that distortion of the DNA might be an energetic barrier to forward progression, and thus a cause for abortive release, Ankit's work is proving this to be false. What you see is not always what you get! Olga Mironova has been developing a novel approach to site specifically labeling our 100 kDa protein, containing 12 cysteines (a more normal approach would be to start with a smaller protein with no cysteines and then introduce a unique one). In this approach, she binds DNA site specifically to the protein, but attached to the DNA is a linker consisting of a cysteine reactive agent, our label (a fluorophore), and a photocleavable

nitrophenyl group. After binding of the DNA and covalent attachment of the cysteine reactive group, she can then photocleave, releasing the DNA and leaving the fluorophore attached to the protein at a unique position. We will use the resulting protein in studies of the large structural change that accompanies the transition from initiation to elongation. Finally, Luis Ramirez has been working on some technologies that will allow us to site specifically label long RNA molecules. This is a new area for us, but one that Luis relishes with a passion! Recent developments on this front have been in collaboration with Prof. Matt Holden in Chemistry. His novel nanodroplet technologies will open up wide new horizons for us. Lastly, Prof. Martin is slowly getting used to the challenges (and excitement) of taking over as Head this past September. It is a daunting, but nevertheless very exciting time, with lots of new possibilities for the Department.

On the alumni front, Rosemary Turingan (PhD '06) is rising through the ranks at Network Biosystems (Woburn, MA), Yi Zhou (PhD '06) is now with Dicerna Pharmaceuticals (Watertown, MA), Eddie Esposito (PhD '05), with Bob Weis and Tony Shrout (PhD '05, Weis), completed an exclusive sublicense agreement with Blue Sky Biotech (Worcester, MA) for the proprietary assay platform invented at UMass Amherst and developed further at Protein Attachment Technology LLC, a company that Esposito, Shrout and Weis founded. Eddie now works at Blue Sky Biotech. After a short postdoc, Xiaoqing Liu (PhD '09) will be returning to China, aiming for a teaching position at home, while Selase Enuameh (PhD '08) has moved from Intelligent Biosystems (Waltham, MA) to a postdoc at UMass Medical School. After about ten years with Nokia in Finland, Charlie Schick (PhD '94) has returned to the USA and is now developing social media (eg, FaceBook) for Children's Hospital in Boston.



Prof. Craig Martin in front of the Molecular Playground.

#### MOLECULAR PLAYGROUND

With an award of \$45,000 from the Camille and Henry Dreyfus Foundation, Prof. Craig Martin and colleagues have created the Molecular Playground, a three-dimensional, interactive display of molecules, ranging from drugs and polymers, to large protein complexes. This Molecular Playground is located in the main atrium of the ISB, where it can be seen and explored by everyone. "Molecules are beautiful," says Martin. "We want to show the 3-D structure of molecules in a way that feels as much like art as possible, while remaining true to the underlying chemistry, so people develop an appreciation for these fascinating structures."

The Molecular Playground is a collaboration with Emeritus Profs. Allen Hanson of Computer Science and Eric Martz of Microbiology, with programming by Computer Science graduate student Adam Williams. The exhibit features colorful 3-D models of well-known compounds such as tamiflu bound to its target protein, the anti-AIDS drug ritonavir bound to the HIV protease, and the natural flavoring acetophenone showing animated IR vibrational modes. The playground will also showcase research at UMass Amherst, such as engineered proton wires being developed in the Chemistry Department. The images are projected on one of the walls in the ISB atrium, and a shadow-sensing IR camera detects users' hand

motions, allowing visitors to move, rotate and resize the molecular image as desired. The overall aim of the Molecular Playground is "to capture the public's attention and to prod individuals to explore personally a vast array of molecular structures in a human-size model." Please explore the playground at its new web site: http://MolecularPlayground.org

#### In the Metz lab ...

In 2009 the Metz group traveled far and wide to study metalligand complexes. Professor Metz went to Orsay, France, using the free-electron laser facility CLIO to study how binding to



The Metz group 2010.

M<sup>2+</sup> influences the C-C and C=O bonds in acetone by measuring vibrational spectra of M<sup>2+</sup>(acetone)4 in the fingerprint region of the infrared. Back in Amherst, **Abdulkadir Kocak** joined the group. Following up on a molecule originally observed by **Fernando Aguirre** (PhD '02), **Abdulkadir** and

Geoff Austein-Miller (Junior undergraduate) measured the rotationally resolved electronic photodissociation spectrum of Co<sup>+</sup> (H<sub>2</sub>O), determining the Co<sup>+</sup>-H<sub>2</sub>O bond strength. They also determined the geometry of the complex from the rotational structure in the spectrum and measured the O-H stretches by combining vibrational excitation in the IR with photodissociation in the visible. Jennifer Daluz (Senior undergraduate) and John Gao (Sophomore undergraduate) also joined the group. Jennifer is building a new metal cluster ion source, and John is carrying out simulations to improve the mass resolution of our photofragment spectrometer. Gokhan Altinay and Prof. Metz carried out a series of photoionization studies on gold-containing compounds at the Advanced Light Source (Lawrence Berkeley National Lab). A highlight was measurements of the ionization energies of gold carbonyls, as well as gold-hydrocarbon complexes. Gokhan has also measured vibrational and electronic spectra of intermediates of oxidation of methane to methanol by CoO+.

#### In the Rotello lab ...

2009 was a busy (and crowded) year in the Rotello lab. Mrinmoy De and Bappa Samanta both received their PhDs and headed west to Northwestern, while Partha Ghosh moved to the coast to postdoc at Yale. Brian Creran was the recipient of an IGERT fellowship, David Solfiell was awarded a CBI training fellowship, and Sarit Agasti received a prestigious Graduate School Fellowship. Professor Rotello was made a Fellow of the American Association for the Advancement of Science, and was appointed as Executive Editor of Advanced Drug Delivery Reviews. It was a record year for publications with 31, one more than 2008. A partial tally includes one in Nature, one in Nature Chemistry, one in the Proceedings of the National Academy of Sciences, one in Nature Materials, two in Nano Letters, one in Angewandte Chemie, and three in the Journal of the American Chemical Society.

#### In the Schnarr lab ...

It has been an exciting year with the Schnarr Lab now in full swing. Jon Amoroso and Lawrence Borketey, now third year graduate students, have made significant headway toward engineering and discovering new drug molecules in bacteria. Both are expecting to publish their preliminary work in the very near future. Carrie Dulaney has finished her Master's Thesis work and will graduate at the end of spring semester. Two new graduate students, Gitanjeli Prasad and Tsung-Yi Lin, joined the lab and are running full swing with their respective projects. Gitanjeli comes to us from India and Tsung-Yi from Taiwan. Star undergraduate, Cornelius Taabazuing, was awarded an EXROP Fellowship from the Howard Hughes Medical Institute to do summer research at the University of Colorado under Professor and Nobel Laureate, Tom Cech. He has since been admitted into our graduate program and will begin working with Prof. Mike Knapp this spring. Christine Okwesili, Mylorde Cherenfant, and Nguendab Gwanyalla have all joined the group as undergraduate researchers from the biochemistry department and are learning the ins and outs of working at the interface of chemistry and biology. With these additions, the lab is bustling with activity.

Professor Schnarr continues to teach graduate organic courses and will add a special topics course in biosynthesis to his teaching resume this spring. He will have his first experience in a large-lecture setting this coming fall when he teaches undergraduate organic chemistry for non-majors. Professor Schnarr was also recently accepted into the Molecular and Cellular Biology (MCB) graduate program as a full faculty member and can begin recruiting students from that program in addition to chemistry, which should further diversify his research group. Last but not least, Nate and his wife, Lindsay, have made it through their first year of marriage and continue to explore everything that the Northeast has to offer in terms of food, culture, and natural beauty with any and all available free time.



The Schnarr group 2010.

#### In the Thayumanavan lab ...

The Thayumanavan group enjoyed another productive year in 2009. Below are some of the highlights of the group. Please

visit us also at http://www.umass.edu/thaigroup for more on our news and achievements. If you are a group alum and we do not have your updated whereabouts, please let us know.

Graduate student update: The group welcomed Diego Amado Torres, Andrea Della Pelle, Raj Rami Reddy, and Feng Wang early in 2009. Also, Judy Ventura is continuing as a chemistry graduate student in our group, after completing her NEAGEP internship in the group. The group is also hosting Warathip Siripornnoppakhun for one year under the Royal Thai Scholarship from Chulalongkorn University in Thailand. Raghunath Roy, after finishing his PhD, is now a postdoctoral associate with Thomas Epps in the Chemical Engineering Department at the University of Delaware. Akamol Klaikherd started as a product development scientist at the Siam Modified Start in Bangkok, Thailand. Yangbin Chen recently took a position in Itaconix Inc. in New Hampshire. Malar Azagarsamy was honored as one of the graduate students to present his work at the annual Chemistry Department ResearchFest. Tejaswini Kale won a prestigious Isenberg Fellowship from the School of Management.

Undergraduate student update: Pardeep Thandi and Dan Terk started Med School at UMass Worcester. Dave Waterman, after graduation, took a break with family in Las Vegas; won some significant amount of money (Dave did not reveal the amount); and went around the world with his sister for a long vacation with the money. More recently, Dave accepted a position in a research lab in Harvard Med. Keith Barbato, Sean Bickerton, and Juna Jovani are continuing to work in the group, along with newcomers Tal Aharon, Brendan Nagle, Sangjin Nam, and Edd Ricker.

Postdoctoral associate update: K. Krishnamoorthy took an independent position at the National Chemical Laboratory in Pune in India. Sunita Satav and Punidha Sokkalingam returned to India after two years in the group. Shreedhar Bhat, Prakash Babu, Sreedhar Reddy, and Anupat Potisatityuenyong joined the group.



Thai's group, along with their significant others, enjoying their 2009 holiday party.

Thai was given the Conti Faculty Fellowship for the year 2009-10 by the University. The group has developed a new block copolymer that is simultaneously sensitive to multiple

stimuli. This work was published in the *Journal of the American Chemical Society (JACS)*, and the work was further highlighted by the *Royal Society of Chemistry* and the *JACS* image challenge. In collaboration with the **Hayward** group in PSE and **Tuominen** group in Physics, the group has demonstrated that the nanoscale confinement of proton transport functionalities in polymers results in significant enhancement in proton conductivity. The research groups have filed a patent because of the potential commercial implications. This work is being supported by the Fueling the Future Center for Chemical Innovation.

#### In the Thompson lab ...

It's been a good year in the Thompson lab, with a variety of projects that seek to understand and harness membrane proteins, including bacterial chemoreceptors, an ABC transporter, and the M2 proton channel. Congratulations to Dan Fowler who defended his PhD thesis in January! Dan completed a challenging study combining NMR and biochemistry to investigate structures of active signaling complexes of chemoreceptors, with a surprising and important result. He was selected to present this work in a talk at the CBI retreat in June and has just published a paper on it in Biochemistry. Dan is now pursuing a joint postdoctoral position with the Hardy and Thompson labs with the goal of engineering proton conducting membranes with M2 channels for fuel cell applications. Fe Consolacion is completing a biochemical study of chemoreceptors reconstituted into membrane vesicles, to investigate the role of receptor clustering in the signaling mechanism. Seena Koshy has developed a mass spectrometry-based hydrogen exchange method for measuring dynamics of chemoreceptor cytoplasmic domains within active signaling complexes. Her results demonstrate that assembly of the active complex significantly reduces receptor dynamics. She can now use this novel approach to compare global dynamics of different signaling states, and then local dynamics of different parts of the receptor, to address longstanding questions regarding the role of protein dynamics in signaling. Shiela Jones has just returned from a Winter School on Biomolecular Solid State NMR. She has engineered a much more efficient expression/purification system for preparing chemoreceptor proteins, to enable her to use NMR to map interface contacts between the proteins in the active array. We had help from two undergraduates on chemotaxis projects this year, Derianne Jeffeke, a SPUR student last summer, and Adam Nelson, a Chemical Engineering major who joined the lab this fall.

Several undergraduates in the lab investigated how the energy of ATP hydrolysis powers transport of methionine across membranes by an ABC transporter. **Ngoc Ho** completed her BS in Biochemistry in May and joined the graduate program at UMass Worcester. **Max Leabo** continued **Ngoc**'s efforts to prepare active methionine transporter reconstituted into vesicles during the summer. **Chris Vercollone** added

a crystallographic effort to his biochemical project on this transporter as an Amgen Scholar last summer at Caltech, in the laboratory of **Doug Rees**, and is back continuing his work as a senior this year.

In alumni news, it was great to catch up with Eleonora Del Federico (PhD '00) when she gave a seminar at Smith College last spring on her work using NMR and other methods in art conservation. Eleonora is an Associate Professor at the Pratt Institute in Brooklyn and does research at the Metropolitan Museum of Art.



The Thompson group, 2010.

Professor Thompson is happy to have just completed submission of the competitive renewal proposal for the CBI Training grant. She is also a co-PI for two new programs at UMass Amherst, a Postbaccalaureate Research Education Program (PREP) funded by NIH for under-represented groups in biomedical sciences, and a mutual mentoring program for UMass Amherst women faculty in life sciences, funded by a Mellon Foundation grant.

#### In the Tyson lab ...

In the Tyson lab, one new graduate student, Nan Wang joined in January to lead our work on atomic fluorescence spectrometry. Senior graduate student James Kearns was awarded a Fellowship by the Indo-US Science and Technology Forum and Oak Ridge Associated Universities Research



presenting the plaque to Prof. Tyson.

Internship in Science & Engineering (RISE) program, and he worked at the Indian Institute of Chemical Biology Kolkata and the Central Glass and Ceramics Research Institute for a period of about three months before visiting Thailand and Vietnam.

International links with Thailand and Turkey were further fostered by visits by Prof. Tyson in January and June, respectively. Both visits involved plenary lectures at conferences, visits to several universities, and workshops (with Prof. Holly Davis) on writing scientific English. Professor Tyson received a commemorative plaque from a member of the Thai Royal Family, Prof. Dr. Her Royal Highness Princess Chulabhorn, and has photographs to prove it. Miss Sirinapa (Mai) Wongwilawan, a top undergraduate student from Naresuan University in Thailand, where former student Dr. Wipharat (Jum) Chuachaud is a faculty member, has been working at UMass Amherst for a few months on the determination of mercury in rice.

Graduate students Tiffany Berg, Monique Johnson, Chengbei Li, and Lindsay Drennan have all successfully completed their dissertation prospectuses and original research proposals. Monique was awarded an IGERT Fellowship from the MassNanoTech Institute. The Tyson group is still providing support for the water analysis lab of the Environmental Institute, with Chengbei providing the leadership.

Undergraduate students Paul Nardi, Drew Smith, Bejan Hakimi, Nick D'Eramo and Claudine Mapa worked on arsenic-related projects in the spring, and we had a summer group of Paul, Neil Desai, Peter Duffy and Jonah Zimmerman from UMass Amherst and Brian Cooper (an REU student) from Lincoln University. In the fall, Neil continued and was joined by Bejan, Drew, Peter, Andrew Craig, and Gloria Chan (who worked with Lindsay and Mai on the mercury project).

Faculty members Peter Uden (emeritus), Ray D'Alonzo (adjunct) and Ed Voigtman, continue to make welcome inputs to group activities.

Professor Tyson and Davis have co-authored, with Jan Pechenik of Tufts University, "A Short Guide to Writing About Chemistry" that was published by Pearson Education Inc. in December. An article based on Dr. Khalid Alassaf's work on arsenic speciation in soils was featured on the cover of the April issue the Journal of Analytical Atomic Spectrometry, and a major paper describing Dr. Christopher Palmer's work on the speciation of selenium and sulfur by simultaneous atomic fluorescence and molecular emission spectrometries appeared in Analytica Chimica Acta in October; this issue also featured the work of Dr. Prince Amoako on the formation of dimethyldiselenide in selenium-enriched dietary supplements. The arsenic-in-soil paper garnered considerable national and international press coverage. An article (in the Journal of Hazardous Materials) on the determination of lead in wine and rum by a flow injection-hydride generation-atomic absorption spectrometry method developed by Prof. Dr. Latif Elci and Prof. Zikri Arslan was featured on the SpectrocopyNow.com.

Congratulations to former graduate student **Dr. Chey Kahakachchi**, who is now the father of **Milan Kavith Kahakachchi** and is working for Covidien in Hazelwood MO, and to **Prof. Wipharat Chuachaud**, who is now married. Prof. Tyson can be found on LinkedIn.com, and, if you look hard, even on facebook.com. He is now the associate dean for academic affairs of the newly created College of Natural Sciences (http://www.cns.umass.edu/). Check it out.

#### In the Vachet lab ...

Professor Vachet and his lab had another busy, productive, and successful year. Particularly exciting news was the successful funding of two proposals, an NIH renewal and a grant from the NSF. Each grant has money for the purchase of new equipment, so in early 2010 the group will receive two new mass spectrometers. 2009 was also a good year for science as the group published six papers and made 18 presentations at various conferences and meetings.

In other group news, Andrea Gomez Escudero was selected to be one of the four speakers at the Chemistry Department's annual Research Symposium in September. She was also honored with the Rohm and Haas/Dow Award for her talk. In the Spring, Emma Downs finished her BS degree in chemistry with Honors, and she is now a graduate student in Environmental Chemistry at the University of Oregon. Guanshi Zhang finished his Master's degree and hopes to soon start a new program in Biomedical Engineering. We were also pleased to host Mario Barón-Rodríguez for four months last year. Mario is a graduate student in Cristian Blanco's (PhD from Auerbach in 2004) group at the Universidad Industrial de Santander in Bucaramanga, Colombia and brought some expertise in protein computational modeling. We also welcomed four new members to the group – Jia Dong, Bo Yan, Yuping Zhou, and Kol Fatunmbi. Jia, Yuping, and Kol are developing new mass spectrometric methods to further our understanding of  $\beta$ -2-microglobulin amyloid formation. **Bo**, who is jointly advised with Prof. Rotello, and is developing new methods to detect and characterize nanoparticles in cells.



The Vachet group, 2009.

In alumni news, former group member **Jon Wilson** (PhD '05) began a new position as Senior Mass Spectrometry Applications Scientist at Perkin Elmer after many successful years at Bruker Daltonics. **Michelle Herrmann** (MS '00) started at new job at the National Cancer Institute in Maryland after many years living in San Diego, CA. **Myra Callaway** (MS '03) is now working at the Albert Einstein College of Medicine alongside former labmate **Jihyeon Lim** (PhD '04), who is a Research Professor in the Department of Pathology there.

Finally, Prof. Vachet was very busy professionally. He taught his annual two-day short course on Quadrupole Ion Trap Mass Spectrometry at the American Society for Mass Spectrometry meeting in June, was named to the Editorial Board for the *Journal of the American Society for Mass Spectrometry*, was a member of the Scientific Advisory Board for the International Conference on the Environmental Implications and Applications of Nanotechnology, and was recently elected to be a member of the Board of Directors for the American Society for Mass Spectrometry.

#### In the Venkataraman lab ...

The DV group had another great year. **Dipankar Basak** received the *Peter Lillya Award* for outstanding poster presentation in Researchfest 2009. The award includes a monetary reward of \$250. The group welcomed **Kedhar Jhadav** and **Dana Algaier** into the group. Our pro/con debate format for discussing literature was published in the journal *Nature*. The group's research focus has change a little



bit over the past year. The group is getting back to the studies on helicenes. Our efforts in the area of photovoltaic cells have started to bear fruit. We have learned a lot about the issue of packing and the role of molecular architecture in organic photovoltaic cells. For some of the recent research news, check out our group website.

With regard to alums, Jason Field (PhD '03) is now a Senior Sector Advisor for the Life Sciences in the Ministry of Economic Development and Trade for the Government of Canada. Jay and Lora welcomed Dylan in April 2009. I understand from Jay and Lora that Rebecca is a proud big sister. Derek Van Allen (PhD '04) is at US Naval research laboratory. Uche Anyanwu (PhD '05) is with Momentive (formerly GE). Craig Bates is now a Senior investigator at Arqule. Craig, Gemma and big brother Isaac welcomed Evan in Nov 2009. Rattan Gujadhur (PhD '03) is still with Gilead as Manager for Strategic Outsourcing. Pranorm Saejueng (PhD '06) is a faculty at Ubonrajathanee University in Thailand. She is pursuing her research in copper-based

cross-coupling reactions. Travis Benanti (PhD '08) is now at Solarity in PA. Travis and Nora welcomed Lillian in September. Nestor Chevere-Trinidad (PhD '08) is at Heatbath Corporation in Indian Orchard, MA as a Chief Research Scientist. Tom Hill left Cytec Industries in Springfield and is now Senior Product Development Chemist at Flexcon. I heard that Gordon Smith (BS '07) obtained a Master's degree from UCSB and is working in CA. Jocelyn Scheintaub (BS '06) finished her Masters from UC Berkeley and has moved to the Seattle area. To my surprise, I got a note from Jocelyn from Ooty in India! She was apparently visiting India with Mike. Dan Burke (BS '06) is also at UCSB working with Prof. Craig Hawker. Jackie Murphy (BS '04) is now a postdoc with Greg Fu at MIT. Noah Tremblay (BS '04) graduated from Prof. Colin Nukolls' group in Columbia and is now a postdoc at Johns Hopkins with Prof. Howard Katz. Thomas van der Poll (BS '09) works for Prof. Gui Bazan at the UCSB. I would like to hear from all the alums from the DV group. So keep me posted.

#### In the Voigtman lab ...

During the spring, 2009 semester, I taught CHEM 112 in the brand new ISB. I had 300 students and it was VERY intense, but fun! What a great building and showcase! Sorry about the Silver Tree spill! I moved to a new office (Goessmann 167) and put my stamp on it, replete with a laser table for detection limit experiments with violet laser diodes. Then this past fall semester, I taught a 185 student section of CHEM 112. So maybe I'm finally learning this stuff! I also continued as an associate head, while Craig Martin made the jump to Department Head in September, and as graduate program director until New Year's Eve. I have another paper in the works (maybe more) and it is exciting to see the department growing even during a down cycle in the economy. Best of success to us all!

#### In the Weis lab ...

First-year graduate student **Meili Yang** has joined the lab to work alongside **Aruni Karunanayake**, who plans to finish in May. **Meili** is advised jointly with **Prof. Igor Kaltashov** and continues investigations into the assembly and function of proteins in the *E. coli* chemotaxis signaling pathway. **Lubna Al-Challah** has completed experiments on the regulation of expression on Geobacter PilA. **Lubna** is writing her dissertation and manuscripts at Cornell, where her husband, **Hanno Richter**, is a research associate.

Several Weis-lab alums have remained in (or returned to) the Bay State. Following graduation **Hoa Tran** (PhD '09) took on a research fellowship at Massachusetts General Hospital. A stones-throw away in Cambridge, **Anas Chalah** (PhD '05) is Director of Instructional Laboratories in the School of Engineering and Applied Sciences at Harvard (http://yardmagazine.harvard.edu/liters-to-lasers/). To satisfy his

need for speed, Anas now owns the red Porsche that was just a screen-saver in graduate school. After venturing west, both Xianhua Yi (PhD '02) and Laila Kott (PhD '02) returned east to Cambridge. Xianhua made use of his 'solid training in protein chemistry' to master mass spectrometry as a postdoctoral fellow with Michael MacCoss (University of Washington), and then joined Momenta Pharmaceuticals (Cambridge) as a Staff Scientist in 2007. Laila landed on her feet after the Pfizer Ann Arbor facility closed – as a Senior Analytical Chemist at Ash-Stevens (Detroit, MI). But never one to stand still or content to follow where others have trod, Laila also plied her skills as an analytical chemist and microbiologist to ferment gourmet wine and vinegar on the northern shores of Lake Erie. Nonetheless, she could not resist the call east and joined Millenium Pharmaceuticals as a Senior Scientist. Across the Charles, Tatiana Besschetnova (PhD '06) is delving more deeply into systems biology to study the mechanisms of vascular malformation as a Research Fellow with Bjorn Olsen (Department of Cell Biology, Harvard Medical School) after finishing a postdoctoral fellowship with Jagesh Shah in the Department of Systems Biology. Tanya's work there is published in Nature Genetics and Current Biology. Anthony Shrout (PhD '06) rounds out the alums in the Bay State to an even half dozen. Tony teaches chemistry at the high school in Longmeadow; a move that came as P.A. Tech merged operations with Blue Sky Biotech, which develops and markets kinase assays based on P.A. Tech's technology, for use in highthroughput screening of drug candidates against membraneassociated protein targets (http://www.blueskybiotech.com/).

Alums in other states and countries include Frances Antommattei (PhD '05), Abdalin Asinas (PhD '07), David Montefusco (PhD '07) and Li Zhi (MCB '05). Frances, who now believes that 'time flies', lives and works in Cincinnati, OH. Frances advanced to Senior Scientist at Procter and Gamble after three years and will be with the company five years in June 2010. On a personal note, Frances and her husband Bob are happy parents of Anna Marie, who was born April 2009. Abdalin resides in 'Toronto the Good', where she is a postdoctoral fellow with Sirano Dhe-Paganon in the Structural Genomics Consortium (Univ. Toronto). David has stayed on the signaling path as a postdoctoral fellow with Yusuf Hannun in the Department of Biochemistry and Molecular Biology at the Medical University of South Carolina, Charleston. David's research seeks to 'define pathways of sphingolipid-mediated cell regulation'. After postdoctoral work in the Laboratory of Immunology at NIAID with David Margulies, Li moved across the NIH campus to join the FDA as an ORISE Fellow (an entry-level scientist) in the Laboratory of Cellular Hematology at the Center for Biologics Evaluation and Research. Li may have thought that she and her family escaped New England snows after moving to the DC area; perhaps climate change had other plans.

### RETIREMENT

#### **Professor Dave Adams Retires**



When Dave Adams walked into his organic chemistry lecture on Friday, December 11, 2009, he was met by the collective applause of his students and many of his colleagues plus a cake to celebrate the formal end of

his distinguished career in teaching and his immeasurable contributions to UMass Amherst. After the celebration, Dave made a few remarks about his experience as a teacher and then got on to what he does best, teaching chemistry. Dave arrived at UMass Amherst in September 1963 when this was a more intimate place with fewer than 10,000 students. He remembers going to Friday night pep rallies behind the Student Union, knowing several of the football stars personally and watching football games up close from wooden bleachers where the Hagis Mall is now. He knew all his class officers. The UMass Amherst team went undefeated to the '65 G.E. College Bowl, buoyed by large pep rallies and crowds that met the team bus on its return.

The chemistry class of 1967 was a talented group, internally competitive but with abundant group identity and spirit. Professor Marvin Rausch introduced Dave to research in his sophomore year. That summer he did research in Rausch's laboratory, supported by a small stipend and living in a basement room in the Amity St. house of classmate, Bruce Colby. On graduating, he turned down a good offer from General Electric and with his wife Lynne, a chemistry classmate, went to the University of Connecticut where he earned a PhD in the laboratory of Wyman Vaughan. His next experience, as a teaching postdoctoral fellow at Penn State, convinced him that teaching was his passion. So again he turned down more lucrative offers to accept a job at North Shore Community College in Beverly, MA.

Fourteen years at North Shore included eight years as Assistant, then Associate, Dean of Academic Affairs and 3.5 years providing evening instruction in organic chemistry at Salem State College. Offered a full deanship at another college, Dave chose instead to return to full-time teaching at the small four-year school, Bradford College in Haverhill, MA where he served as Chair of the Division of Natural Sciences and Mathematics. He recalls this as one of the most creative periods in his career. After three years at

Bradford, Dave moved to Babson College in Wellesley, MA where he continued to excel in developing chemistry courses for non-science students and to teach nights at Harvard extension. Most characteristic of Dave's teaching was its quality. He won teaching awards both at Babson and Harvard.

### *in*MEMORIAM

#### Remembering George Oberlander



Prof. George Oberlander teaching in Peter's Auditorium, Goessmann Laboratory.

When George James Oberlander died on 6 July 2009, we lost a friend and colleague who contributed to the development of today's Department in manifold ways. Throughout most of his

UMass Amherst career, George served in a dual role – heavily involved in department logistics and administration and serving as a mainstay in the large faculty group that taught thousands of students in general chemistry courses. He began as a teacher and, as his career matured, assumed administrative responsibilities serving as the Department's "Director of Laboratories" from 1970 to 1979. In this role he made major contributions to planning of the Lederle Graduate Research Tower.

George was a native of Boston, served in the USAAF from 1942 to 1946 and finished his interrupted BS in chemistry at Tufts University in 1947. He worked briefly at Stone & Webster Engineering in Boston, taught chemistry to returning veterans at Fort Devens and then joined the UMass Amherst faculty to teach laboratories and eventually lecture in General Chemistry. He completed an MS degree in chemistry at UMass Amherst in 1955; his thesis research was directed by Prof. J. Harold Smith. Two black-bound copies of his MS thesis entitled "A Study of the Complexes of Iron (III) With Phenols and Enols in Aqueous solution" reside in the UMass Amherst Science Library. Some of you who took the "Qual Organic" course may remember using ferric chloride solution to test for phenols and enols. Formation of colored complexes is the basis of this test.

Following his retirement, George and his wife, Jennie continued to live in their College St. house in Amherst while they indulged their love of travel visiting Canada, Mexico, the Caribbean, South America, and much of the US. George was an avid Red Sox fan and lived to see his faith redeemed though he had to wait for a new century for it to happen. He kept in shape by swimming at the Hampshire Fitness Club. George and Jennie eventually moved to Burlington, VT to be closer to family. George was a vital presence in the General Chemistry complex in Goessmann Laboratory, stocky, with a ruddy round face, impatient and bursting with energy. He was one of those colleagues who helped make a career in chemistry at UMass Amherst so satisfying. —Peter Lillya

## Marion Rhodes (1923-2009) –Remembrances



Marion was only two months short of 10 years of her very active retirement as Emeritus Professor when she passed away on November 11, 2009 after more than 50 years associated with the UMass Amherst chemistry department. Not everyone realized that Marion had continued to teach her beloved

course in Optical Chemical Microscopy at least once a year in retirement until fall 2008. Generations of graduate and some undergraduate students had benefited from her highly personal style of hands-on instruction in what was virtually a tutorial laboratory class. It was a particular pleasure to her that alumni often commented how valuable the course had been and that optical microscopy, seldom seen in graduate analytical chemistry programs, had been helpful in their own careers. On hearing of her death, a recent graduate commented "I took two of her courses, she was a great teacher and it was a pleasure to listen to her many enlightening stories!" Marion was delighted that a modern purpose-built microscopy laboratory had been established for her work.

Born in St. Louis, Missouri, she nevertheless became a true New Englander, never more so than when she designed her post-and-beam retirement home and forest refuge in Sunderland on the western slopes of Mount Toby. In an alternate career track Marion might well have pursued her passion for botany and ecology, a pathway that circumstances did not permit as she pursued her academic pathway. In retirement she volunteered in promoting the activities of the renowned Smith College Botanic Garden. Marion had a great love for African Plants and it was particularly moving that at her graveside funeral service in the peaceful Riverside Cemetery in Sunderland, a fine floral tribute of exotic and African flowers was the centerpiece.

Marion spent many of her early years in Connecticut earning her BS in chemistry at UConn while working nights in the textile mills of Willimantic. Marion's early academic career involved instructorships in the UConn system both in chemistry, but also in the agronomy and genetics departments. Her association with UMass Amherst began first as an analytical chemist at the Feed and Fertilizer Experiment Station, and she also obtained her MS in physical chemistry in 1960. Her academic career in UMass Amherst Chemistry was established with her doctoral research (PhD '66) in the burgeoning field of polymer physical chemistry under the direction of Dick Stein. She moved through the academic ranks from Instructor to Professor (1989), teaching mostly in the general chemistry program for some 20 years before moving to focus in analytical and physical areas. She maintained a broad research program in polymer morphology throughout her career, publishing more than 50 papers primarily on the structural analysis of polyurethane foams utilizing optical microscopy.

An example of the way in which Marion combined her personal avocation and her professional focus was as a gifted photographer. She was an accomplished botanical and nature photographer and enabled many students to develop their own skills in the context of her photomicroscopy teaching.

Marion was never one to be disinclined to take on new ventures, and I offer one personal example. In 1995 she was invited to travel to Xiamen University in southeastern China to present a graduate course in chemical microscopy. UMass Amherst had developed a strong link there, and since I had spent time there on two occasions, I was able to encourage her to grasp this opportunity. She relished her visit there and despite initial trepidation she counted it one of her finest professional experiences.

To quote from her obituary; 'Marion lived the philosophy that the only way to implement change was to be part of the solution – to the very end, Marion did it her way.' –*Peter C. Uden* 

### 2009 SEMINAR SERIES

The UMass Amherst Department of Chemistry seminar program draws renowned scientists from around the globe to our campus to share their insights and recent developments. Our department hosted 23 seminars this past year, and some of the highlights included seminars from several distinguished speakers.



Professors Bryan Coughlin and Richard Schrock

Each spring the UMass Amherst and Smith, Mt. Holyoke, Amherst and Hampshire Colleges collaborate to host the *Five College Lecture Series*. For 2009, we were fortunate to host **Prof.** Richard Schrock from the Massachusetts Institute of Technology. Although Prof. Schrock is well known for his work in olefin metathesis, which netted him a share of the 2005 Nobel Prize in Chemistry, his lifelong interests in inorganic chemistry have focused on another Nobel-worthy project. Turning nitrogen gas into ammonia (a key ingredient of nitrate fertilizers worldwide) on an industrial scale is carried out by the age-old and energy hungry Haber process. In his seminar "Reduction of Dinitrogen to Ammonia under mild conditions" **Prof. Schrock** remarked that nature performs the same reaction to the scale of 300 million tons per year using nitrogenase

metalloenzymes. He then excited our audience with his recent advances in trying to create a non-biological equivalent of the catalytic metalloenzyme center to enable dinitrogen to ammonia conversion under mild conditions.

In April, our department was also graced with a visit by UMass Amherst alum (BS '55) **Prof.**Richard Holm from Harvard University as a part of a new *Distinguished Chemistry Lecture Series*. **Professor Holm** is one of the leading inorganic chemists in the world, and he spoke to us about his synthetic, structural, and reactivity studies of metal-sulfur clusters, which comprise the active sites of many important enzymes such as nitrogenase, carbon monoxide dehydrogenases, and ferrodoxins. Enzymes with such clusters carry out some incredibly important and difficult chemical transformations, and for decades chemists have been trying to understand and mimic this chemistry by creating synthetic analogs. **Professor Holm**'s seminar described his recent work in this area and some of the beautiful complexes his group has been able to make, characterize, and study.



Professors Richard Holm and Michael Maroney



Professor Emeritus Richard Stein and Dr. Cady Coleman

The 2009 Stein-Bayer Lecture Series, named after Prof. Emeritus Richard Stein and sponsored by Bayer MaterialScience, was a homecoming for another UMass Amherst alum, Dr. Cady Coleman, who received her doctorate in Polymer Science and Engineering in 1991. Dr. Coleman is a NASA Astronaut and a Colonel in the US Air Force. As a scientist-astronaut crew member of two Space Shuttle missions, she shared her perspective the on past, present and future of space experiments in her talk "Getting Materials Science off the Ground." She also highlighted the capabilities of the International Space Station (ISS) as a scientific laboratory by describing ongoing work in fluid physics, colloid science, and crystallization, and reminded the audience that the ISS is intended to be a user facility much like US national labs. Finally, Dr. Coleman talked about her training and

preparation for her November 2010 launch and subsequent six month stay aboard the ISS. You can follow **Dr. Coleman**'s training on CNN's American Morning series, "Counting Down Cady" or at http://amfix.blogs.cnn.com/category/counting-down-cady/.

This year's *William E. Mahoney Seminar* lecturer was the Chancellor of the University of California at San Diego, **Dr. Marye Anne Fox**. **Dr. Fox** became involved with university administration following an outstanding career as a leading physical chemist. In her seminar "The Troubled Future of American Public Higher Education," **Dr. Fox** explained how California's financial crisis made relying on state funding for education and research unsustainable. As alternatives, she described how federal and private sector partnerships can be created and used to both maintain university operations and in some cases invigorate new research. In particular, green energy partnerships promise to be beneficial for UCSD and the energy industry. **Chancellor Fox**'s message reached beyond UMass Amherst Chemistry, as the audience also included several key UMass Amherst administrators, including **Chancellor Holub**, **Provost Staros** and several college Deans.



Mr. William Mahoney and Chancellor Marye Anne Fox

The 2009 seminar series ended with a visit from Prof. Amit Meller from Boston University, who was our *Procter & Gamble Seminar* speaker. In his talk "From DNA capture to DNA sequencing using solid-state nanopores," Dr. Meller provided a fascinating tour through his recent work in the area of nanotechnology. By using a nanometer-sized pore just slightly bigger than the width of a DNA molecule, Dr. Meller has created an incredibly sensitive DNA detector. Dr. Meller described how

#### 2009 SEMINAR SERIES...-continued

his strategy could be used to detect genes and possibly sequence DNA. With the completion of the human genome project and the personal genome sequencing on the horizon, **Dr. Meller** treated the audience with a glimpse of how very small technology might lead to a very big medical revolution.

The success of this year's UMass Amherst Chemistry seminar program was made possible through the generous contributions of our alumni and corporate sponsors. The students and faculty are immensely grateful for the unique interactions and opportunities for learning and enrichment that the alumni and sponsorship support provides.



Professors Ray D'Alonzo and Amit Meller

### **RESEARCHFEST 2009**

The Chemistry Department welcomed the academic year 2009-2010 with the 19th annual research symposium, Researchfest. The event was held on September 1, 2009 and was a huge success thanks to the the support of participants, organizers and sponsors. The event featured four oral presentations by the graduate students; the presenters were selected by a faculty committee through



Malar Azagarsamy, Andrea Gomez, Oscar Miranda, and Kevin Early

nomination/evaluation process. Kevin Early (Barnes Group) was chosen to receive the first Richard K. and Meryl M. Brown Graduate Scholarship in Chemistry of \$5,000 for his work on "Polarization Spectroscopy of Single Quantum Dot Emitters." Malar Azhagan Azagarsamy (Thayumanavan Group) received the Procter and Gamble Award for "Enzyme Triggered Disassembly of Dendrimer based Amphiphilic Nanoassemblies," Andrea Gomez (Vachet Group) received the Rohm & Haas/Dow Award for "Using Amphiphilic Polymers to Selectively Extract and Concentrate Peptides for Analysis by Mass Spectrometry," and Oscar Miranda (Rotello Group) received the William E. McEwen Fellowship Award for "Chemical Nose" Sensors: Identification and Detection of Proteins, Bacteria and Cancerous Cells."

A total of 48 posters were presented in the event surpassing the number of posters from the past researchfest events. The following four students received awards for outstanding posters:

William E. McEwen Fellowship Award for Outstanding Poster sponsored by: Dipankar Basak (DV Group) for "Impact of Molecular Motions on Proton Transfer."

Peter C. Uden Award for Outstanding Poster sponsored by P&G: Sravanti Vaidya (Hardy Group) for "Structural and Biochemical Studies on the Role of Prodomain and Linker in the Activation of caspase-6."

William E. McEwen Fellowship Award for Outstanding Poster: Ankit Vahia (Martin Group) for "Evidence Against Scrunching as a Mechanism for Abortive cycling in RNA Polymerase."

William E. McEwen Fellowship Award for Outstanding Poster: Myoung-Hwan Park (Rotello Group) for "Chemically Directed Immobilization of Nanoparticles on Silica/Gold Substrates via Dithiocarbamate Bond Formation."

A whole day with Chemistry and scientific discussions was brought to an end with a delicious BBQ served in ISB amphitheater by the graduate students C. Subramani, Brian Creron (Rotello Group). The BBQ brought the students, faculty, staff and their families together to socialize.

We gratefully acknowledge the financial support we received for this event from UMass Amherst Department of Chemistry, *Richard & Meryl Brown Scholarship Fund*, *William E. McEwen Endowment Fund*, *Rohm & Haas*, and *Procter & Gamble*. –Student Development Committee

## undergraduate SENIOR & AWARDS DINNER



Professor Paul Lahti and the 2009 Senior Class.

Each spring the Undergraduate Honors and Awards Committee has the pleasure of examining the records of those students that have chosen to be a part of our Department. Each spring, we honor those students that have proven themselves to be among the very best this University has to offer. And so we did last May at our annual Undergraduate Honors and Awards banquet. At this banquet, we recognized the hard work and dedication of over 20 graduating seniors. In addition, over 30 students were recognized for their work within the Department (see the complete list below). These awards are only possible because of the generous support that the Department receives from our alumni, industrial partners and professional organizations. And so, the committee wishes to thank the students for their contributions to the Department and University and those that, in turn, support our students.

The following students received awards:

Pardeep Thandi – Connecticut Valley Section of the American Chemical Society (CVS/ACS) Student Award Thomas S. van der Poll – American Institute of Chemists

Award

*Emma L. Downs and Brittany J. Chaney-Ryan* – Richard W. Fessenden Award

**David Waterman and David Mortenson** – Merck Index Award

**Thomas S. van der Poll and Pardeep Thandi** – Senior Class Award

Alicia Wood – Departmental Recognition Award

Tamara Allen – John A. Chandler Memorial Scholarship

Award

**David Mortenson** – Hypercube Scholar Award **Malek Mazzawi** – ACS Analytical Chemistry Award **Ed Cooke** – Jay A. Pirog Scholarship

Peter Duffy, Juna Jovani, Abdullah Majidi, Artem Maksov, Jamal Salah and Carolyn Tieu – Edward Shapiro Scholarship Kevin Johnson, Margaret-Mary Morelli, Margaret Reid and Emily Twaalfhoven – Robert Maxwell Williams Memorial Scholarships

Kathryn Geldart, Srinivasa Gopolsamy, Jason Lee and Dylan Lovinger – CRC Freshman Chemistry Award Michelle Boisvert, Dennis Kim, Alan Stebbins and Matt Stevens – Honors General Chemistry Poster Award Malek Mazzawi – Oliver T. Zajicek Undergraduate Scholarship

Sean Bickerton – Bates Research Fellowship

Joseph Ryan – Bradspies Research Fellowship

Tamara Allen and Sean Bickerton – Hach Fellowship

Margarita Antonov, Elliott Ethridge and Pardeep Thandi

- Outstanding Undergraduate Researchers 2009

## degrees AWARDED

BA/BS DEGREES				PHD DEGREES	
Samuel B. Bearg	02/2009	Daniel G.Terk	02/2009	Rochelle Arvizo	05/2009
Kevin P. Chan	05/2009	Pardeep S.Thandi	05/2009	Adrienne Carver	09/2009
Brittany J. Chaney-Ryan	05/2009	Jimmy C.Tran	05/2009	Nestor Chevere-Trindad	02/2009
Emma L. Downs	05/2009	Charles C. Wainwright	02/2009	Mrinmoy De	05/2009
Elliott M. Ethridge	05/2009	Alicia M.Wood	05/2009	Priyanka Dobriyal	02/2009
Alex G. Jackson	05/2009			Agya Frimpong	09/2009
Christopher S. Johnson	02/2009	MS DEGREES		Partha Ghosh	09/2009
Steven Joubanian	09/2008			Brian Jordan	02/2009
Mary C. Kociuba	05/2009	Martha Azuero	02/2009	Xiaoqing Liu	09/2009
Manvi Madhok	09/2008	Jinhong Kim	09/2009	Michael Murphy	02/2009
David E. Mortenson	05/2009	Guanshi Zhang	09/2009	Arpornrat Nantalakul	02/2009
Timothy G. Mortsolf	05/2009	Gdaristii Zharig	07/2007	Ruthanne (Hassey) Paradise	09/2009
Paul A. Nardi	05/2009			Manori Perera Gunawardhana	02/2009
Jerahmy L. Parsons	05/2009			Raghunath Roy	09/2009
Quoc Hung V. Pham	05/2009			Elamprakash Savariar	02/2009
Erin L. Sutherland	05/2009			Hoa Tran	09/2009

### newADDITIONS



Matt Holden and Min Chen welcomed Neil Chen Holden on September 29, 2009 to their family. He was 19.7 inches long, and his weight was 6 lbs 7 ozs.

Max Lein (Maroney group) and his wife, Gina, are proud to announce the birth of Evelynn Brenya on January 28, 2009. She was 21 3/4 inches long, and her weight was 7 lbs 6 ozs.





Dhandapani (DV)
Venkataraman and his wife,
Meera welcomed their son,
Ashwin, on April 23, 2009.
He was 8 lbs 9 ozs and 20
inches long. Shreya is being a
proud big sister.

## staffCHANGES

This past summer, after many many years of working in the Chemistry department, **Mark Snow** finally succumbed to the temptation and retired. As everyone knows, Mark has been the one who has helped keep the department running all these years. His willingness to do whatever it takes to get a job done, his ability to perform miracles and his excellent attitude will be surely missed.

Mark has been a dear colleague to many of us in the department. He has deservedly earned the reputation of not only being a hard worker, but also being creative in his approaches to solving a problem. All of us have benefited from Mark's significant assistance over the years.

Thankfully, he'll still be in the area working in his family's new establishment, "Snowzees" up on Route 116 (Sunderland). He welcomes everyone to stop by and say hi.

Fortunately, we were able to hire to fill the vacant position and we welcome **Ryan Feyrer** once again to our department. Ryan previously worked with us managing our Stockroom and most recently was working over in the Campus Center. Ryan has already begun to make a positive impact and we are happy to have his enthusiasm and strong work ethic back with us.

## *it*UPDATE

As of the end of 2009, Chemistry/BMB's three-member IT team supports over 1,000 computers and 70 network switches across a three-building network. Over the past year we have made substantial upgrades to the network in preparation for deploying VLANs (virtual networking) which will allow us to provide much greater flexibility to our users while also substantially increasing the security of the network; currently we successfully block or otherwise circumvent between eighty to a hundred thousand attempts to compromise our departmental servers each and every day. It will also allow us to support the deployment of wireless networking, which we anticipate will happen in early 2010. We also pioneered implementing Access Grid, a multi-site conferencing system designed to integrate not just lecturers but entire audiences across multiple remote locations.

Our largest project over the past year has been the opening of the Integrated Sciences Building and the outfitting of the new Computer Resource Center. Chem/BMB IT played a pivotal role in not only bringing the networking environment live, but configured and deployed four new servers to provide services to the users of both the CRC and the entire building. We have created a whole new system of managing users and groups via LDAP that is groundbreaking not just at UMass but unique across the world, and that meets not only the needs of Chemistry and Biochemistry & Molecular Biology but is also a substantial step forward towards a truly collaborative relationship with Biology and eventually other departments within the College of Natural Sciences. Comprising over 30,000 lines of programming code and still growing as we expand the new system's ability to provide and support additional tools and resources, this is a critical piece of the Chem/BMB infrastructure.



We anticipate 2010 will see the final deployment of VLANs and the addition of further functionality to our custom LDAP services, as we continue to provide timely services to our user community. We also hope to make upgrades to several aging servers, and as our budget allows to move forward with implementing more robust file storage and backup/disaster recovery solutions. – IT Team

## Impressive New Building is a Great Place to Learn

The opening of the Integrated Sciences Building (ISB) in January 2009 was eagerly anticipated, and this new state-of-the art teaching laboratory and lecture space has lived up to all the initial excitement. Now that ISB has been in use for a full year, we thought you might appreciate how this new building has enhanced teaching and learning in the Chemistry Department. So, we asked Peter Duffy, a senior chemistry major from Northampton, MA, Prof. Justin Fermann, and Prof. David Sommerfeld to provide their perspectives on the fantastic new building.

#### A STUDENT'S PERSPECTIVE



Peter Duffy

The Integrated Science Building is nothing short of impressive. During the Fall of 2009, I had the opportunity to express this feeling to the new College of Natural Science advisory board only days after joining the student leadership committee. The first thing I shared was that the ISB provides students with exactly the learning environment and tools necessary to facilitate a quality education. I also

explained that the ISB honors teachers and staff by providing excellent multimedia classrooms, bright offices, new safe laboratory spaces, and a generally enjoyable and useful facility to teach in. As someone who has long been familiar with the UMass Amherst campus and who has many family alumni of UMass Amherst, I have been impressed by what the ISB has to offer current and future students.

My personal experiences over the last year, I think, give a glimpse into what the building has to offer. Upon entering the ISB for the first time, I found the architecture reminiscent of many of the campus' newer structures. The ISB has a large open atrium with an entire wall of windows to let in natural light, and plenty of lounge space to sit and study on every floor. This is a world of difference from the narrow darker hallways of older structures on campus, which often have no place to commune with fellow students.

At the beginning of the school year last fall, the new College of Natural Science was able to host a barbeque for the thousands of students just outside the building. As part of the student leadership committee I donned the standard issue maroon shirt with UMass Amherst logo and catchy saying, and helped hand out ice cream at the event. Students and guests, however, were left wondering where the trash cans were. The ISB is so high speed that I had to direct people to the trash and recycling bins built into cubbies in the wall, cleverly camouflaged as building decor. Small details like the trashcans may pale in comparison to features like the Mo-

lecular Playground, which is a projected interactive molecule display in the atrium, but they help me appreciate the building even more. Of course, the ISB provides temperature controlled lab space with plenty of hoods to work in and easy access between wet labs and instrumentation, with well thought out floor plans. The laboratory areas even include lounge space outside to provide comfort while waiting for class to begin.

While recently giving a presentation for class, I was able to use the aforementioned Molecular Playground in the ISB atrium. I was presenting the drug Tamiflu (Osiltamivire) as a potential candidate for chemical compound of 2009. The interactive display showed how Tamiflu inhibits influenza and allowed students to rotate and view the molecule as desired. The ISB has many useful features like this that enhance our education. The most prominent of these features may be the Computer Resource Center (CRC). The CRC is equipped with several flat screen Mac computers, useful chemistry software, printing, and break out cubicles for tutoring. I have spent many long hours in the CRC working on chemistry homework and lab reports with other students. In the CRC it is rare that anyone turns on the lights. I like it that way, and I don't know why; I think most students feel the same. This is where I would like to point out how dedicated the ISB and UMass Amherst students are to environmental concerns. The ISB was designed with an awareness of its environmental impact. I figure the students are reflecting that initiative in their energy conservation efforts.

As a commuter student I enjoy the time I spend on campus at the ISB. It provides a relaxing, dynamic environment in which to study between classes and a convenient location to meet with on-campus students. Many chemistry professors have offices in the building, and their offices are very accessible and convenient for office hours. Often I have gone in search of one professor for assistance, and if he/she was not available I found someone else who was. They would see me hovering outside in the communal office area and invite me in for a chat. Having such ease of access to the faculty is reassuring because it means guidance is always available.

Just like the faculty, the ISB will be available to help out students for years to come. As I have said, the facilities are

#### IMPRESSIVE NEW BUILDING...-continued

nothing less than impressive, and I am quite grateful to have them at my disposal during my time at UMass Amherst.

–Peter Duffy (BS '10)

#### CRC in ISB

One of the most important, but often overlooked, contributors to student confidence and motivation is the learning environment. The ISB in general, and the CRC in particular, have shown students that UMass Amherst prioritizes their education and has put in the effort and resources to provide a world-class science building solely dedicated to the education of undergraduate students. Their feeling of ownership of the learning space, and participation in decisions about its function and use, engenders a positive and energized attitude to learning.

The CRC is used as a drop-in hub for individual study, student team learning, informal education, and collaborative work. Computers in the CRC have software that supports student projects from on-line intelligent tutoring in introductory science classes to research-grade analytical,



Chemistry Resouce Center (CRC)

mathematical, and computational chemistry tools. Break out rooms encourage peer-led team learning, and full north wall natural light helps minimize fatigue - at least during the day! A variety of work environments are provided and used, including computer equipped round tables, partitioned meeting rooms, stepped classroom seating, arrangeable and fixed furniture, and board and projection space. Students choose and use the space best suited for their activities.

Small, computer-enhanced classroom environments provided by the "wing rooms" just off the CRC get used for formal instruction at all levels of undergraduate education, generally in the mornings when there is lighter drop-in use. These rooms provide the ability to "teach with technology." By using in-class specialized computer software a different kind of learning can occur than in a traditional lecture. By working with data, exploring phenomena using simulations, or using research tools to ask and answer their own ques-

tions, students work on the skills of being a scientist, rather than knowing scientific facts.

Having research tools - specifically quantum chemistry molecular modeling software - available in an exciting learning environment has really awoken a sense of discovery in some students. For example, Thomas Foley, a current sophomore, found a passion for research investigation through his experiences using WebMO in Chem 121 and followed up with a 1-credit colloquium on electronic structure. On his own initiative, he began investigating the weak acid nature of HF by performing an impressive series of water cluster calculations with embedded H+, X-, and HX species (X = F, Cl, Br). He has demonstrated trends in  $\Delta H$  and  $\Delta S$  for the aqueous ionization of these species and has sought a molecular-level explanation for the qualitatively distinct behavior of HF. His work is presently being written up as a computational chemistry educational exercise and will be submitted to the Journal of Chemical Education. In the classroom students at all levels are now being exposed to - and are embracing - the computational, analytical, and visualization tools that are prevalent in research.

- Professor Justin Fermann

#### WORLD-CLASS TEACHING LABS

A year after moving into the ISB, I still marvel at the facility and the changes it brought and continues to bring to our mission. Though the move from my office in Goessmann to my new office in the ISB was only 200 meters, it was also a move of 50 years. Those who took Physical Chemistry here in years past no doubt fondly remember Goessmann 128; the drafts that came in under the window sills, the sweltering temperatures of late spring and early fall semesters, the inadequate hood space and the patched and varied floor. Now you walk into ISB 355A and see a clean, open, well-lit, climate-controlled space with 2 full and 2 half hoods. Then, you look down the building to see...the entire suite of labs. Even though I had been involved in the planning process for this space, its sheer size did not strike home until I walked into ISB 355 the very first time.

The analytical and physical chemistry teaching labs are an open laboratory space with unobstructed lines-of-sight and large windows with a western exposure. On a sunny day, no artificial light is necessary and at times shades must be drawn in order to facilitate the work. Three large teaching labs are separated by two prep labs. In addition, we have an optically isolated room for laser-based experiments. Only the 'wet' lab is set-up as a traditional space with large lab benches suitable for teams of students all working on the same experiment during a given period. The two instrumentation rooms are arranged with six large tables upon which 1-2 instruments can be placed. This new space has energized the students. It



Bill Schmitt teaching in the Organic Lab

is a pleasant place to be. We have enough hood space so that crowding is no longer an issue; no waiting in line for a balance; and the lab dishwashers allow us to keep the glassware in a much better state. These are all small matters, but they make for a more enjoyable lab experience, and students can more readily focus upon what they are doing and learning in the lab.

My favorite aspects of the lab space are two areas that allow for 'teaching' moments. Outside the lab, there is semi-private space at the end of the hallway. It has cushioned benches, coffee tables and a black board. This space is ideal for small lab lectures. Within the instrumental labs, there are not any shades; rather, there are white boards set in tracks. They can be opened or closed to control lighting levels and they serve as a wonderful place to give brief explanations regarding a lab and its method, purpose, physical underpinning, and so forth. This is a building that was well designed as a teaching space.

Regarding instrumentation, our facility is now one of the best equipped undergraduate labs in the northeast. We have the capability to investigate material properties (AFM and DSC), biomolecular systems (LC-MS and CE), environmental chemistry (GC-MS and GFAAS) and energy-related chemistry (Nd:YAG laser and pulsed spectrofluorometer). We even have a glove

box for those experiments that require an inert atmosphere for sample preparation and storage. These instruments allow us to expand the scope and types of experiments that we offer Chemistry majors, and most importantly, they will better prepare students for graduate school or a career in chemistry and/or pharmacy. We have the tools and so we are now updating our curriculum to better use them.

The move into ISB is a seminal moment in the history of our undergraduate program. It offers us the opportunity to take this program to the next tier and better prepare our students for the future. This has been a wonderfully hectic year made possible by the generosity of our alumni, the drive and foresight of those that planned and built this facility and the hard work and devotion of our support staff. —Professor David Sommerfeld

#### FUELING THE FUTURE-continued from page 1

The current Phase I center led by Prof. S. "Thai" Thayumanavan includes Chemistry faculty members Scott Auerbach, Michael Barnes, Justin Fermann, Jeanne Hardy, and D. Venkataraman, along with colleagues in Polymer Science and Engineering (Bryan Coughlin and Ryan Hayward), Physics (Mark Tuominen), Chemical Engineering (Peter Monson), and at Yale University (Mark Johnson). Over the past year, the Center has made great strides in understanding charge transport across a molecule-to-materials continuum, chiefly for applications in fuel cells but also in photovoltaic systems.

Several achievements by a multi-investigator team headed by Scott Auerbach have provided fundamental insights into the so-called Grotthuss mechanism of molecular-scale proton transfer. The Grotthuss mechanism, first suggested by Theodor Grotthuss in 1806 to explain the anomalously rapid diffusion of protons in water, can be visualized as a "bucket brigade" used in former times to provide water for putting out fires. Just as buckets are passed along a line of people to move water over great distances, protons can be passed

along great distances through neighboring water molecules. This is precisely how protons are predicted to move through a new class of solid-state proton conducting materials being investigated by Auerbach, Johnson, and Venkataraman. By designing optimum pathways for charge transport through theory and experimentation at molecular length scales, this team is establishing the basic science underlying future high-tech materials for energy applications.

A second team led by Jeanne Hardy and Mike Barnes has used single-molecule studies to determine architectures for efficient charge transport among groups of molecules at the nanoscale. Thus far, a single-molecule research platform comprised of a photo-acid generator attached to either a helical peptide or a rigid linear monomer scaffold, linked in turn to a pH-sensitive fluorophore, has been utilized by this team. Recent studies have allowed this team to select the optimal scaffold, photoacid generator and fluorophores for these studies. Continued research by this team on new systems of molecular building blocks for charge transfer down "proton wires" and within organic photovoltaic

#### FUELING THE FUTURE-continued from page 24



materials will have great impact in targeting the most advantageous chemicals for tomorrow's energy innovations.

On the bulk materials scale, a third team led by Sankaran "Thai" Thayumanavan has focused on polymer systems. In studying

conducting pathways in polymers, the team's (Thayumanavan, Hayward, and Tuominen) research indicates that polymer morphologies can affect proton conduction. For example, "comb" nanostructures, involving phase-segregated polymers combined with non-conducting decyl chains, were found to exhibit significant proton conductivity, despite the presence of "non-conducting" decyl chains within the solid state polymer assembly. This team has also developed methods for rapid modular fabrication of block copolymers that are used in the model macroscale systems under study and methods for incorporating functionalized charge transport polymers within membrane nanopores to study their impact on nanoscale confinement. The future impact of this fundamental chemical research at the bulk scale will eventually be seen in new classes of technologically-superior nano-engineered organic materials that can be commercialized by industry.

#### ENERGY FRONTIER RESEARCH CENTER-continued from page 1

**GG:** What are the main goals of the Center? **PL:** Basically, to increase the efficiency of organic-based photovoltaic devices well above the present 5-6% conversion, by structural and morphological control strategies, using organic polymers, large molecular chromophores, and organic-inorganic composites.

**GG:** How is the EFRC different than other energy-related centers on campus?

**PL:** The Center does not have an explicit educational component and does not have an explicit goal to produce a "widget." The goal is multi-disciplinary, team-enhanced basic research that could be used in making better photovoltaic devices. So, we will pursue applied testing of the research from EFRC, but application is not the primary goal. The DOE's intent to promote our EFRC basic research is strongly indicated by the fact that ours was one of those funded through the American Recovery and Reinvestment Act (ARRA), meaning that we got all of the Center funding up front.

**GG:** What is your role in the EFRC?

**PL:** I am a researcher in Energy Research Group (ERG) 1, whose primary focus is making new materials (synthesis). Such new materials go to ERG 2 for morphological assembly and study, and thence to ERG 3 for characterization of physical properties (charge-flow efficacy, overall solar spectral conversion efficiency, and test device fabrication). I am also co-PI and co-director of the center, with Silvio Conte Professor of Polymer Science and Engineering **Tom Russell**. Tom and I are responsible for oversight and administration of the center, including frequent reports to the DOE.

**GG:** What other faculty from the Chemistry Department are involved in the Center?

PL: In ERG 1, the Chemistry faculty are Vince Rotello, "Thai" Thayumanavan, D. Venkataraman (DV), and me along with three faculty members from Polymer Science and Engineering (PSE). In ERG 2, DV, who is the cocoordinator of this ERG, is the only Chemistry faculty member involved, but we will have contributions from other faculty on and off campus, including faculty from PSE, Chemical Engineering, and Physics. The off-campus collaborators include scientists from the University of Pittsburgh, Penn St. University, and Oak Ridge National Laboratories. ERG 3 is co-coordinated by Mike Barnes and will include contributions from DV, me, and faculty in PSE and Physics. This ERG also has collaborators from UMass Lowell, Konarka Technologies, Inc., and the National Renewable Energy Laboratory.

**GG:** How will the Center influence the education of our students?

PL: There has been a lot of excitement engendered by the news that the EFRC was funded. The Center does not have a specific education component. That said, everything that is actually done in the lab (that's the good thing about Chemistry; it is a "do it" science) is a learning experience. In particular, the overt team approach that is being developed in EFRC is much like teams that exist in many industries and research centers that pursue multidisciplinary work in modern times.



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Dear Alumni and Friends of the Department of Chemistry,

A new year with lots of changes! After seven very productive years as Head, and with great appreciation from the Department, Bret Jackson stepped down as Head in September. He has left big shoes to fill, but has also left the Department in very good shape. Despite tight budget times, Chemistry has been thriving and we are currently searching for two new faculty: one in the general area of inorganic and one in the area of chemical biology. Our college has recently grown, with the establishment of a new College of Natural Sciences (led by Dean Steve Goodwin), including our old college, plus most of the College of Natural Resources and the Department of Psychology.

At the College awards recognition ceremony in September, Chemistry was featured in every category: Jeanne Hardy won a Lilly Teaching Fellowship to develop a new general education course in forensic chemistry, Mike Maroney won the College Outstanding Research Award, Justin Fermann won the College Outstanding Teacher Award, Marvin Ellin and Vicki DeCarli won the Dean's Service Award, and Paul Lahti won the College Outstanding Service Award. Together with Tom Russell in PS&E, Paul also received a highly competitive \$16M Energy Frontier Research Center grant from the Department of Energy. Indeed, energy research in the Department is thriving, as Thai Thayumanavan not only received the Samuel F. Conti Faculty Fellowship award this year, but has followed up his previously awarded Phase I Center for Chemical Innovation grant with a phase II submission, requesting \$20M over the next five years (renewable to \$40M over ten years) and involving numerous faculty outside of and within Chemistry. Associated with that program, Jeanne Hardy appeared on the WGBY (PBS) program EcoExchange to discuss her contribution, designing peptides as components of hydrogen fuel cells. We are clearly an energetic group of faculty!

This past year has seen the opening of the Integrated Sciences Building, featuring state of the art teaching laboratories, lectures halls, and the new Molecular Playground. The transition of our teaching labs to this building has freed up space for research, some of which we are renovating (from the ground up) with a \$7.4M grant from the National Institutes of Health.

We continue to be deeply grateful to all of you who have contributed so generously to our department over the years. In addition to improving our teaching and research facilities and providing scholarships to students, your gifts help us to provide startup packages for new faculty. With your support, we will forge ahead pushing the frontiers of knowledge and training top-notch students in Chemistry!

Sincerely,

Craig/Martin, Department Head

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