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EVENTS for 2014

Marvin Rausch Lectureship Prof. Tobin J. Marks Northwestern University February 27, 2014

Five College Seminar Prof. Dennis A. Dougherty California Institute of Technology April 3, 2014

Senior Awards Dinner April 30, 2014

Alumni Reunion 2014 June 7, 2014

ResearchFest 2014 August 2014

Stein-Bayer Seminar in Polymer Chemistry Prof. David A. Tirrell California Institute of Technology October 2, 2014

William E. Mahoney Annual Lecture Prof. A. Paul Alivisatos University of California Berkeley November 13, 2014



UMass Amherst Chemists Move into State of the Art Laboratories



The year 2013 will go down as nothing short of momentous for the life sciences research community on campus. Many of the Chemistry Department faculty have benefited from the 'happenings' of this year. First, we saw the completion of construction of a wonderful new research building—the Life Sciences Laboratory (LSL), with move-in taking place in mid-August. Several Chemistry faculty and their research groups are now housed in the LSL. In addition, the campus received a grant of \$95M from the Massachusetts Life Sciences Center (MLSC) to support the establishment of an Institute of Applied Life Sciences (IALS). Approximately one-third of these funds will enable fit-out of the second half of the LSL, where a number of new core facilities

Getting to Know Our Newest Faculty Member

INTERVIEW WITH PROFESSOR MICHELLE FARKAS (MF), recent

hire in organic and chemical biology (BS, Wellesley College, PhD, Caltech; Postdoc, UC Berkeley)

GG: Where did you grow up? MF: Mahwah, NJ

GG: When did you realize you loved chemistry?

MF: I don't know-it was just something I never grew tired of, and there was always



YOU ARE ALL INVITED TO Chemistry Alumni Reunion 2014

The 2014 Chemistry Alumni Reunion will be held on Saturday, June 7, 2014 in the beautiful Integrated Sciences Building (ISB). We will once again be honoring two of Chemistry's towering figures, **Professors George Richason**, **Jr.** and **Richard Stein**, people who have created much of the excellence that is Chemistry at UMass Amherst. This event is part of the university-wide Alumni Weekend.

We are planning the following schedule of events, open to all alumni, students, faculty, staff, and friends.

2-3 pm - Reception for Professors Richason and Stein in the ISB Atrium

3-4 pm - Concurrent Events: General Chemistry Talk and Research Talk

4-5 pm - Reception for Professors Richason and Stein in the ISB Atrium

Check out what the University has planned for alumni weekend as well. Go to http://umassalumni.com/alumni-weekend/

Please RSVP by calling or emailing our Alumni Coordinator, Carrie Morrison Penland, at 413.545.2585 or carriemp@chem.umass.edu. Starting in April you can also register online at http://umassalumni.com/alumni-weekend/register/

We look forward to seeing you in June 2014!





alumninews



Raegan Grace Herbst born July 31, 2012 to **Meaghan Germain** (PhD '08, Knapp) and **Bob Herbst** (PhD '10, Maroney).

Robert J. Snyder (BA '67) retired after a 36 year career. After graduating from UMass Amherst, he went to St John's University in Queens, NY, graduating with a PhD in Physical Chemistry in 1976. His schooling was interupted for a three year stint in the US Army (1968-1971) including a one year tour in Vietnam. Upon receiving his PhD, Dr. Snyder taught for 12 years at Sacred Heart University in Bridgeport, CT; six years of Customer Training at Perkin Elmer Corporation in Wilton, CT; and for the last 18 years, taught at Southern Connecticut State University in New Haven, CT. He retired June 1, 2012 as a full Professor of Chemistry. Dr. Snyder would love to hear from other alumni at robertjsnyder2010@gmail.com.

Dr. Augustine Silveira (PhD '62, with Earl McWhorter), BS '57, ScD (Hon) '75 UMass Dartmouth, was invited as the speaker at the American Chemical Society, Syracuse, NY Section, *Education Night* on June 12, 2013. *Education Night* honors outstanding students and teachers at high school and university levels in Central New York. The title of Dr. Silveira's talk was "Follow Your Dreams—Careers and Opportunities in Chemistry."

Dr. Silveira, Distinguished Teaching Professor Emeritus, retired in 2000 after 37 years in the Chemistry Department at the State University of New York (SUNY) Oswego. He was invited to give the commencement address and was the recipient of the Samuel Stone Lifetime Alumni Science Achievement Award at UMD in 2007. He also gave the commencement address and received an Honorary Doctorate of Science degree at SUNY Oswego in 2010.

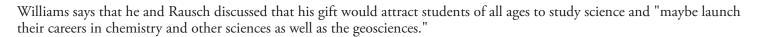
marvin & jane rauschmineral Gallery

The Marvin and Jane Rausch Mineral Gallery has opened with more than 200 spectacular mineral specimens, many rare and unusually large. The gallery also includes a collection of fluorescent minerals, many of which have not been displayed before.

Marvin Rausch, a long-time organometal-lic chemistry professor, donated his entire collection to the University before his death in 2008. According to his wishes, part of the collection was sold to fund an endowed lectureship in Chemistry, but the best were given to the Geosciences department, to establish a collection to serve and educate our students in perpetuity.

The size and color of the specimens makes them particularly attractive, says geologist Mike Williams, a professor in the Geosciences department. "Rausch's collection was certainly regarded as one of the best in New

certainly regarded as one of the best in New England if not in the whole country."



Williams add that the extraordinarily beautiful specimens will entice "students in looking deeper into where they come from, how they're made, and why they grow in these extraordinary shapes."

The new gallery is located in 243 Morrill II Science Center and is open to the public Monday through Friday. There is also a nicely placed window into the gallery that allows appreciation of the highlights 24/7, and a video display containing student-generated explanations of the origins, morphology, and chemistry of the minerals in the collection.



Crocoite

Lead chromate mineral (PbCrO $_4$). This sample comes from the Red Head Mine, Dudas, Tasmania, Australia. Abundant masses with exceptional examples of crocoite crystals have been found in the Adelaide, Red Lead, West Comet, Platt and a few other mines at Tasmania; they are usually found in long slender prisms, usually about 10–20 mm but rarely up to 200 mm (4 inches) in length, with a brilliant lustre and color. Crocoite is also the official Tasmanian mineral emblem. (Wikipedia)



Wulfenite

Lead molybdate mineral (PbMO $_4$). The wulfenite in the sample occurs with black mottramite. Most often found as thin tabular crystals with a bright orangered to yellow-orange color. It occurs as a secondary mineral in oxidized hydrothermal lead deposits. This specimen came from the "79 Mine", Dripping Springs Mountain, near Hayden, Gila County Arizona. (Wikipedia)

POINTS of PRIDE in Chemistry

- Michael Barnes renewed his Department of Energy research grant "Chemical Microscopy of Conjugated Polymers"
- Michael Barnes was selected to receive the 2014 John
 Burlew Award from the American Chemical Society's
 Connecticut Valley section (CVS). This award recognizes
 Mike's pioneering research in single molecule spectroscopy.
 He will be the featured keynote speaker at the 2014 CVS
 Undergraduate Research Symposium which will be held at
 UMass on Saturday, April 26, 2014.
- Lila Gierasch has been selected to receive the 2014 Mildred Cohn Award in Biological Chemistry, awarded annually by the American Society for Biochemistry and Molecular Biology (ASBMB).
- Jeanne Hardy has received a Fulbright Scholar award from the Council for International Exchange of Scholars to pursue her research on Alzheimer's disease.
- Jeanne Hardy won the seventh annual Armstrong Fund for Science Award, which this year is granting \$30,000 over two years to encourage transformative research that introduces new ways of thinking about pressing scientific or technical challenges.
- Matthew Holden received a NSF CAREER Award for his research on "Revealing the Mechanism of Non-endocytotic CPP-modulated Protein Delivery."
- Kevin Kittilstved recently had an invited manuscript accepted for the "2014 Emerging Investigators" themed issue of the *Journal of Materials Chemistry A* (a publication of the Royal Society of Chemistry).
- Chemistry seniors Kate Liedell and Michael Veling were honored at commencement on May 10, 2013, for being named 21st Century Leaders and for their far-ranging achievement, initiative and social awareness.
- Vincent Rotello brought low-cost, inkjet-printed nano test strips to Pakistan for drinking water tests.
- Vincent Rotello has been named the new editor-in-chief of *Bioconjugate Chemistry*.
- Sankaran Thayumanavan's polymer nanogels were highlighted by UMass in their Research Next.
- Diego Amado Torres (Thayumanavan group) was awarded one of the top 5 best poster presentations (from over 170) in the Colloids and Surface Chemistry division in the ACS meeting held in New Orleans on April 7-11, 2013.
- Guanbo Wang (Kaltashov group) attends the 63rd Lindau Nobel Laureate Meeting in Chemistry.
- Jack Welch (former CEO of GE) comments on how Prof. George Richason's remarkable teaching changed the trajectory of his life in an April 20, 2013 article of the Boston Globe.
- Graduate student Jiaming Zhuang (Thayumanavan group)
 was awarded an extremely competitive and prestigious
 Graduate School Fellowship.

labnotes

In the AUERBACH LAB ...

Diels-Alder?

Ring opening?

The Auerbach group had another wonderful year in 2013 with several articles published in Biofuel Production, Fuel Cell Materials, and Inorganic Network/Zeolite Formation—all from a theoretical chemistry perspective. Particularly noteworthy is an article summarizing research led by Auerbach-lab postdoc **Dr. S. Vaitheeswaran** ("Vaithee") in collaboration with Chemical Engineering professor **Paul Dauenhauer** and his PhD student **Sara Green**. The article—entitled "Biofuels from Furan: Discriminating Diels-Alder and Ring-Opening Mechanisms," and published in *ACS Catalysis*—clarifies the detailed mechanism by which biomass

converts to biofuels inside zeolite nano-cavities. In particular, when biomass is rapidly heat-

ed (undergoes
"fast pyrolysis")
it produces
pyrolysis
vapors, which
enter into the
shape-selective nanopores of

acid zeolites for further "biore-

finement." The basic question we asked is this: what exactly happens during this biorefinement?

Answering this question can help to improve and scale-up "catalytic fast pyrolysis" as a way to provide cellulosic biofuels to millions of Americans. Although many investigators have hypothesized that Diels-Alder chemistry dominates the biorefinement process, the Auerbach team surmised that zeolite pores may be too confining to allow such chemistry, especially between the bulky cyclic organics that arise during pyrolysis. Our work, which is a combination of computational chemistry modeling and experimental reaction engineering, found indeed that an alternative "ring-opening" mechanism is likely in play. We are continuing work on this, applying quantum chemistry to compute the zeolitecatalyzed barriers for this process for comparison with experiment, to ensure we have complete understanding of how to make biofuels from biomass. Dr. Vaitheeswaran is still at UMass Amherst, continuing his research on biofuel production, and also teaching Quantum Chemistry to Chemical Engineering undergraduates.

Professor Auerbach remains the founding director of the Integrated Concentration in Science (iCons) Program. This exciting integrated science program for undergraduates is now in its fourth year, with the "student pipeline" full, and with a senior cohort of "First Class" iCons scholars poised for great things after graduation. For more information on iCons, please see the update on page 18.

In other exciting news, Prof. Auerbach bumped into former Jackson-group student, now Prof. Joseph Quattrucci at Worcester State University, when Prof. Auerbach was running a workshop on building iCons case studies for integrative science courses. Prof. Quattrucci remains hard at work teaching General and Physical Chemistry, and also continuing his research into computational the theoretical surface science of carbon, graphene, and carbon nanotubes. We all wish Prof. Quattrucci the best in his endeavors, as we do for all alums of the Auerbach-Jackson "CRUNCH" Lab (Chemistry Research Using Nice Computer Hardware:).



Professors Auerbach and Quattrucci at WSU.

In the BARNES LAB ...

In the past year, Prof. Mike Barnes continued research supported by the US Department of Energy on "Chemical Microscopy of Conjugated Nanomaterials" and successfully renewed this grant totalling \$420,000 (through 2016), and the Polymer-based MRSEC at UMass Amherst. In addition, he was co-investigator and team leader on the US Department of Energy EFRC at UMass led by Profs. Tom Russell and Paul Lahti.

Barnes also was named recipient of the 2014 John Burlew Award from the Connecticut Valley Section of the American Chemical Society.

Our group members and research news:

Adam Wise, a postdoctoral researcher in our group, was involved in multiple projects including ultrafast transient absorption experiments on crystalline polymer nanowires, chemically cross-linked nanowires, and oriented single crystals of small-molecule organic semiconductors.

Kevin Early (PhD '10) "Photophysics of hybrid quantum dot-conjugated organic nanostructures") is now at 3M Corporation in Minneapolis, MN where he heads the Quantum Dot Display laboratory.

Austin Cyphersmith (PhD '12) "Probing effects of orientation on the chiroptical properties of single molecules") completed a postdoctoral assignment at Georgia Tech, and is now at Princeton Instruments.

Mina Bahghar, now a 5th year Physics graduate student is working on near-field imaging and Raman spectroscopy of polymer nanostructures.

Joelle Labastide, now a 4th year Chemistry graduate student, continued her thesis work on time-resolved photoluminescence studies of oriented crystalline polymer nanowires. Joelle also received the *Richard and Meryl Brown Scholarship for Excellence in Research*—the top graduate prize in Chemistry at UMass—for her work on time- and polarization-resolved fluorescence studies on isolated polymer nanowires.

A number of undergraduates have made significant contributions to our group's research efforts over the past year: Derek Maxwell (BS '14), Claire Miller (BS '14), Sandra McEnroe (BS '15).

In the CHAMBERS LAB ...

Over the last year, the Chambers lab has continued working at the interface of chemistry and biology, studying basic problems in neuroscience. Our work on new probes to label endogenous neuroscience receptors has resulted in an overwhelming abundance of data, a few new collaborations including one with a National Institute on Drug Abuse scientist, and some new directions for our molecules.

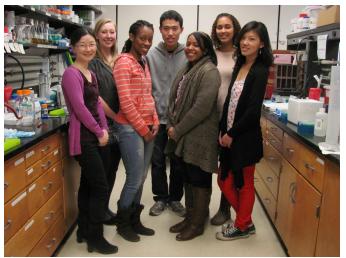
The lab consists of three Chemistry doctoral students, Amanda Hussey, Steve McCarron, and Devon McCarthy, two Neuroscience and Behavior doctoral students, Rosie Combs-Bachmann and Jefferys Nate Johnson, and one Molecular and Cell Biology doctoral student, Kathryne Medeiros. The lab will be sending off a few of these fine students into the world for their next adventures as newly minted PhDs. In addition to the great graduate students, the lab continues to host a number of super-talented undergraduates with majors ranging from Psychology/Neuroscience to Biology to BMB to Chemistry throughout the year.

Up to date info, awards, data, presentations, and other news can always be found at www.chamberslab.com/wp/

In the CHEN LAB ...

The Chen's group continued the work on the functional mechanism of pore-forming membrane proteins and their applications in biosensing and drug delivery.

Monifa (Mo) Fahie, now a third-year MCB graduate student discovered a non-classic assembly pathway of cytolysin A (ClyA) pore forming toxin from *E. coli*. She gave a talk



Chen group 2013.

about her results in the CBI Chalk Talk which won her the best chalk talk award. Her finding was published in the *Journal of Biological Chemistry* last year. Mo will continue to explore this unusual mechanism by which ClyA toxin attack host cells. She has been recently awarded with the UMass Amherst CBI Fellowship to support this project.

Christina Chisholm, a third-year MCB graduate student who has been working on engineering an outer membrane porin OmpG as a biosensor to detect disease-related biomarkers. In collaboration with **Dr. Lukas Tamm**'s group, she recently published a co-author paper about the dynamics of the loops of OmpG in the *Journal of the American Chemical Society*.

We also welcome two new group members: Bib Yang, a Chemistry graduate student who is investigating the molecular translocation though ClyA pores which has implications for nanopore DNA sequencing and drug delivery; Alzira Avelino, a MCB master's student who is experimenting on putting a molecular switch to ClyA which only turns on its functionality at cancer cell surface.

The Chen's lab has celebrated our move to the newly renovated lab on 8th floor. We are excited about the new space and certainly look forward to a more productive year in 2014!

In the **DUBIN LAB** ...

Check out what the group has been up to at **people.chem.** umass.edu/pdubin/dubinlab/

In the GIERASCH LAB ...

2013 was a particularly exciting year at the Gierasch lab. During this year, we said goodbye to very valuable and loved lab members: MCB Graduate student Mylene Ferrolino (after giving birth to beautiful baby Juelle!) presented her dissertation and set off to Memphis, TN to become a

Postdoctoral Fellow at St. Jude Children's Hospital. Almost at the same time, Ivan Budyak left after working several years in our lab as a postdoctoral fellow, to join Eli Lilly in Indianapolis, IN as a research scientist. And during the summer, Anastasia Zhuravleva started her independent career as a faculty member at the University of Leeds, UK, after her postdoctoral work on the Hsp70 chaperone. Additionally, undergraduate student Bradley Quade finished his Honor Thesis in the lab and started graduate school at the University of Texas Southwestern Medical Center. There, he joined the lab Jose Rizo-Rey, who was a member of the Gierasch lab in the early 90's. We miss Mylene, Ivan, Anastasia and Brad very much, and we wish them the best of luck!

In the usual passages of academia, we welcomed a new postdoctoral fellow, Wenli Meng, who did his graduate work with Dan Raleigh in the Department of Chemistry of the State University of New York at Stony Brook. Wenli is an expert in NMR and will apply his knowledge in the study of the Hsp70 chaperone. Also, we hosted undergraduate students from the ICE REU program and high school students who want to start off their careers early on: This year we hosted Maile Hollinger from Amherst College, who presented a poster at the Summer Undergraduate Research Conference (ICE/HHMI) on her research performed in the lab, and high school students Monica Beeferman, Alan Tang, and Dorry Zhao. The lab was very busy and the students had a great summer experience.



Gierasch group 2013.

It was a good year for publications as well: We published two book chapters, three research articles in prestigious journals, and three refereed review articles.

Lila and the group presented our research at several local meetings such as the joint CBI/BMB/BMP retreat with UMass Medical School, and also at national conferences like the Biophysical Society in Philadelphia, PA, the Keystone symposium: Frontiers of NMR in Biology in Snowbird,

UT, the Annual Meeting of the Protein Society in Boston, MA, etc. We also traveled far and wide across the globe, presenting at international meetings like the Annual Meeting of the Swedish Structural Biology Network, Tallberg, Sweden, the International Conference on Systems Biology, Copenhagen, Denmark, and the EMBO Conference on The Molecular Biology of Chaperones, Sardinia, Italy.

The high point of 2013 was the change of venue for the Gierasch lab! The whole lab was packed into boxes over the summer and moved with the help of every single member of the crew. It was a very busy time, but we all had fun and enjoyed the process, saying "goodbye" to Lederle Graduate Research Tower (see picture), and "hello" to the new Life Sciences Laboratories, where you can find us on the third floor. We share our new space with other members of the Biochemistry and Chemistry Departments working on protein folding and diseases associated with misfolding and aggregation of proteins, and the wonderful new space fosters interactions and research collaborations. This research is being greatly enhanced by new industry partnerships and new instrumentation, with the support of the Massachusetts Life Sciences Center grant and our new Institute for Applied Life Sciences.

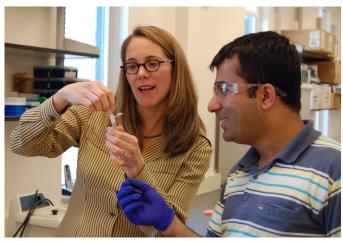
We wish all another year of good science and great fun in the lab!

In the HARDY LAB ...

This has been a great year for the Hardy Lab. In April 2013 we moved into a beautiful, newly renovated lab on the 7th floor of LGRT, adjacent to the lab of Matt Holden. We have been loving our new space and our ability to perform radioactive assays and tissue culture experiments. In the fall we were happy to welcome Michelle Farkas to the floor.

In May, lab alumna Kristen Huber (Signum Biosciences) returned to help us celebrate the graduations of Elih Velazquez-Delgado (St. Jude's Research Hospital) and Samantha Nicholls (Harvard Medical School). This fall Muslum Yildiz published a paper on an allosteric site he discovered in the protease from Dengue virus, which causes Dengue fever, in ACS Chemical Biology, successfully defended his dissertation and was awarded a UMass PhD! He has since returned to Turkey to pursue a postdoctoral fellowship.

Kevin Dagbay was honored as recepient of the 3M Award for Most Outstanding Poster Presentation at ResearchFest this year just weeks after welcoming his first son, Sebastian, into the world. Bay Serrano and Scott Eron both were awarded William E. McEwen Fellowship Poster Awards at ResearchFest, making us one proud lab with three prize winners. Bay Serrano has also been awarded a UMass CBI fellowship for the second year running. Bay and classmate



Prof. Jeanne Hardy and graduate student Muslum Yildiz.

Yunlong Zhou both successfully passed their prospectus defenses. Bay, Yunlong and Scott have made great strides in understanding the battle between kinases and caspases, which is critical to a large number of disease states. We were all impressed that Scott survived his third Tough Mudder race while he made these advances! Our two outstanding second year graduate students Maureen Hill and Derek MacPherson have both hit the ground running. They have each already determined at least one crystal structure and are working on their first paper together. Our awesome undergraduates, Jacob Lytle and John Slatterly have both proven to be exceptionally valuable team members and are well on their way to authorship! Prof. Hardy has spent the fall semester on sabbatical in the lab of Takeshi Iwatsubo and Taisuke Tomita at The University of Tokyo studying the molecular basis of Alzheimer's disease and the role of caspases in disease progression. She was also awarded a Fulbright Fellowship to study the structure of caspase-6 by NMR during spring semester 2014 during her sabbatical at the Pasteur Institute in Paris, France in the laboratory of Muriel Delepierre.

In the HOLDEN LAB ...

To see what's new in the Holden lab, please visit people.chem.umass.edu/mholden/

In the JACKSON LAB ...

Our group continues to explore the dynamics of several important gas-surface reactions, with a focus this past year on understanding methane dissociation on Ni and Pt catalysts. In earlier work, two postdocs, Sven Nave and Ashwani Kumar Tiwari, demonstrated that the observed strong increase in the reaction probability with increasing metal temperature was caused by a variation of the activation energy with the motion of the metal lattice. More recently, we have been able to compute fully quantum dissociative sticking probabilities, as a function of the temperature of the metal and the translational and vibrational energy of the methane. We have completed

studies of methane reactions on Ni(111) and Ni(100) surfaces, as well as the highly-corrugated Pt(110)-(1x2) surface (with undergraduate Dongwon Han). Dongwon graduated last spring (BS Math '13) and Sven and Ashwani are now assistant professors in Orsay, France and Kolkata, India, respectively. This past summer, graduate student Inara Colón-Diaz published a study of how adsorbate coverage modifies the dissociative sticking probability of methane on a Pt(111) catalyst, in collaboration with the Beck experimental group at EPFL. Also this past summer, graduate student Mike Mastromatteo published a study of methane reactions on Ni surfaces using classical mechanics with a reaction path Hamiltonian, before leaving the group with a Master's degree. Two new graduate students, Azar Farjamnia and Han Guo, have joined the group. This work has received a great deal of attention, leading to invited talks at several major meetings in 2013, including the Dynamics of Molecular Collisions meeting, the Dynamics at Surfaces Gordon Research Conference, and meetings in India, Munich and Berlin.

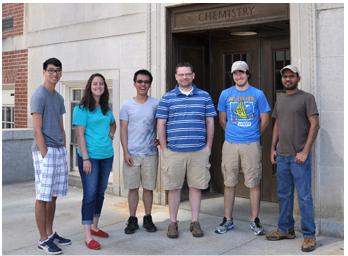
In the KALTASHOV LAB ...

2013 was a very busy year in the Kaltashov laboratory, which included publication of ten papers (including one published in the *Proceedings of the National Academy of Sciences*), filing a patent (US Provisional Patent Application U1188.70011US00: Compositions and methods for delivering agents to the central nervous system) and several presentations given by the group members at numerous scientific meetings and conferences. Two group members defended their PhD dissertations and moved to the University of Utrecht in Netherlands (Guanbo Wang) and Regeneron Pharmaceuticals (Shunhai Wang), and an exceptional graduate student (Xiaofang Zhong) joined the group us in December 2013.

In the KITTILSTVED LAB ...

2013 was a very productive year in our study of the chemistry and physics of transition metal ions in semiconductor nanostructures and oxide materials. Graduate students William Harrigan, Jenileigh Harris and Keith Lehuta have made exciting strides in the study of bulk and nanoscale perovskite materials with potential applications in solid-state memory devices and watersplitting photocatalysts. Graduate students Swamy Pittala and Dongming Zhou have continued studying the interplay of transition metal ions in semiconductor quantum dots and molecular species and we expect to have publications on both projects very soon.

In December, Keith's paper on the speciation of Cr(III) ions during the sol-gel synthesis of SrTiO₃ (strontium titanate, a ferroelectric semiconductor) was published online. This paper is the first from the lab and will be published in an upcoming special issue from Emerging Investigators in the



The Kittilstved Group 2013.

Journal of Materials Chemistry A. This paper highlights our utilization of sophisticated spectroscopies and bulk characterization techniques to understand the mechanism of impurity incorporation into complex materials.

The year ended with the addition of 1st year graduate student Fumitoshi Kato (Western Washington University, '13) to the group. Fumi will be working on controlling the magnetic and luminescent properties of diluted magnetic semiconductor quantum dots with photoactive organic capping ligands.

With increasing numbers, we quickly outgrew the confines of Goessmann (GSMN) 142. We are now also located in newly renovated GSMN 54 (synthetic labs) and GSMN 50 (offices). We are looking forward to a productive and exciting year of research in 2014.

In the KNAPP LAB ...

Go to http://people.chem.umass.edu/knapplab/ to see what the Knapp group has been up to.

In the LAHTI LAB ...

PML was an invited speaker at the North American-Greece-Cyprus May symposium in Limassol, Cyrpus during May 2013, celebrating George Christou's 60th birthday with some excellent science and visits to archeological sites on the historic island. In June 2013, he had the pleasure of presenting an overview of 25 years of work on conjugated polymers with long-time Lahti group collaborator Frank Karasz, at a UMass Amherst 80th birthday celebration and symposium held at Polymer Science & Engineering (PSE). He was also an invited speaker at the International School and Symposium on Molecular Materials in November 2013 at Tokyo Tech, and visiting Waseda University and Keio University during the same trip. UMass Amherst postdoctoral alum Prof. Naoki Yoshioka ('92) has a thriving research program at Keio University, and kindly hosted during that trip. Prof. and Dean Hiroyuki Nishide hosted

the visit to Waseda University, and followed up with a trip the USA to ink a collaborative exchange agreement with the Energy Frontier Research Center at UMass (which PML co-directs with Tom Russell of PSE). The EFRC was highlighted in a recent UMass ResearchNext web publication "Advancing the frontiers of polymerbased photovoltaic research," at https://www.umass.edu/ researchnext/solar-phase. PML also spent a month during September as a visiting professor at Universidade Federal Fluminense (UFF) in Niteroi, Brazil, just across the bay from Rio de Janeiro. The visiting professorship was hosted by Prof. Maria G.F. Vaz of UFF and supported by the Brazilian Ciência sem Fronteiras program, as part of a major collaborative project headed by Prof. Vaz in the area of new magnetic materials. The program has already led to multiple publications jointly between the Lahti group and researchers in the Rio area.

Postdoc Rafael Allão Cassaro received another year of support from CNPq in Brazil to continue his work on molecular magnetism at UMass Amherst.

Graduate student Paul Homnick was selected by the ACS Division of Organic Chemistry to present his work at the Graduate Research Symposium of 2013 at University of Delaware. This is a prestigious and quite competitive selection, and we were very proud to have him present his work about tuning energy levels in conjugated molecules for solar cell work. See Paul at www.organicdivision.org/ama/orig/GRS/GRS2013_GroupPhoto.pdf, just in front of the backmost row, in a blue shirt, second from right to left.

Graduate students **Paul Homnick** (invited ResearchFest speaker), **Jeffrey Lucas** (*William E. McEwen Fellowship Award* for poster) received recognition for presentations of their work at the 2013 Chemistry Department ResearchFest.

Graduate student **Tim Gehan**, jointly in the Lahti and DV groups, has been awarded a prestigious *Isenberg Fellowship*.



PML at Nissan headquarters in Japan.

Tim works on assembling organic semiconducting organic polymers into nanoparticles with controlled size and size distribution. These offer strong prospects to be used in an ecologically low impact, nanoparticle films for solar cells. He aims to use his *Isenberg* opportunity to lean how fundamental research from academic chemistry reaches the real world marketplace.

Alumna Hemali Rathnayake (PhD '07) was awarded tenure and promotion at Western Kentucky University, where her work on making a low-cost, flexible, organic-based solar cell has generated substantial attention and a startup company to pursue commercializing the work: see http://wkunews.wordpress.com/2013/09/9/solar-panel. She, husband Chandana, and children Bhanuka and Hasith are doing well.

Alumnus Burak Esat (PhD '01) sends greetings to UMass from Fatih University in Turkey. His group is doing a lot of work on organic electrode and battery research, including a new collaboration with a Bulgarian institute on batteries through which two of his students worked in Sofia during summer.

Alumus Safo Aboaku (PhD '08) visited UMass during fall, and says that he and his family are doing well in Oxford-MS, where Safo is Instructional Assistant Professor. Son Kofi is now in second grade, and younger daughter Akos is in pre-K. Wife Kate teaches twice a week in the preschool that Akos attends. Work in Olemiss is going well, albet with more teaching responsibilities and increasingly large class sizes. Safo notes that grading of that many scripts in one class can be a challenge.

Alumnus Andrew Ichimura (PhD '92) reports getting through one his busiest seemsters at San Francisco State University, where he has been for 13 years(!). Two students got their MS degrees from his group.

Alumnus Rajdeep Kalgutkar (PhD '01) reports that he is super busy playing a team leadership role on a couple of major projects at 3M, spending much of his time charting paths, getting experiments off the ground and reviewing results.

Alumnus Yi Liao (PhD '01) sends greetings from his new position as Associate Professor at Florida Institute of Technology.

Alumnus **David Modarelli** (PhD '91) sends greetings from University of Akron, but says that he "cannot believe that it's been 27 years now since I joined your group! Egad!"

Postdoc alumnus **Prasanna Ghalsasi** ('01-'02) continues to do well at Maharaja Sayajirao University of Baroda. India

hosted the 2013 International Junior Science Olympiad in Pune, with 39 countries from all over the world (six students per team). **Prasanna** was one of the academic members of the Olympiad, involved in preparing question papers (multiple choice, subjective, and practicals in Physics, Chemistry and Biology), grading, medal awards. The event was for nine days, and preparation took over a year. See http://ijso2013.hbcse.tifr.res.in

Postdoc alumnus Hidenori Murata ('05-'06) is continuing his work on battery-operated cars at Nissan in Yokohama, where he, wife Miho, and their (swiftly growing) children took PML on a tour of Nissan's central headquarters. The Nissan Leaf is very impressive (PML got to zoom in one from Tokyo to Yokahama as part of PML's trip to Japan in November). There are also smaller battery-operated cars available–see photo on page 9.

In the MARONEY LAB ...

The big news from the Maroney lab is that the NIH grant that has been supporting research in aspects of nickel biochemistry for over 25 years was renewed beginning January 1. Anticipation of this funding allowed the group to grow in the fall semester so that it is back up to close to full-strength range. In addition to existing group members Julius Campecino, Carolyn Carr, Heidi Hu (MCB), and Hsin-Ting Huang, postdoctoral researcher Roby Kurian (PhD, Univ. of Maine) and graduate students Priyanka Basak and Zeinab Kaboli have joined the group this fall. The group moved in August from the Lederle Graduate Research Tower to the third floor of the new Life Sciences Laboratories (LSL). Stop in and see the new digs! The tours are free. The life sciences support from the State of Massachusetts will create a new core facility for biophysical characterization of proteins that the group anticipates will make a huge difference to our science. And if that were not enough good news, Prof. Maroney is on sabbatical for the spring semester. Sabbatical plans include finishing two major reviews for a special bioinorganic issue of Chemical Reviews, working on a new collaboration with a new center studying metal ion homeostasis at Durham University in the UK, and lots of travel, including about a half dozen seminar trips around the US.

In the MARTIN LAB ...

Returning from a sabbatical at Caltech in the Spring of 2013, the Martin lab has launched a new initiative aimed at understanding complex folding pathways in large, structured RNAs. You may remember that RNA is the information vehicle that encodes proteins – a disposable, chemical template. The past decade has seen an explosive growth in our understanding of RNA's role in biology – and in us. We now understand that RNA, or a chemical precursor to RNA, was the "primordial" molecule that could both encode itself

and carry out catalysis (and provide mechanical structures). Recent studies have revealed that RNA currently plays key (and previously unappreciated) roles in cellular regulation and catalysis, and adopts complex folded structures. And just as misfolding of proteins can lead to disease states, so too misfolding of structured RNAs has dramatic implications in development, neurochemistry, and just about every other process in the cell. As chemists, we'd like to understand the vast array of noncovalent interactions directing macromolecular folding. One missing tool reflects the fact that large macromolecules fold as they are being synthesized, and sequence-directed pauses in that synthesis are often key to determining different folding outcomes. Using tools from the emerging field of DNA nanotechnology, the Martin lab is developing an approach to mimic this sequential folding of RNA in the test tube, but in a much more controlled manner. We anticipate that this approach will open up new approaches towards understanding the chemistry and biology of the many noncoding, structured RNAs that are only now beginning to be appreciated in biology.

Reporting on recent alums, Luis Ramirez-Tapia (MCB, '13) is now a postdoctoral associate in the laboratory of Carlos Bustamante in the Chemistry Department at the University of California, Berkeley, where he is developing single molecule approaches towards studying life's molecular machines. Satamita Samanta (PhD '12) is a postdoctoral associate in the laboratory of Beverly Emerson at the Salk Institute (and UCSD), and studies the regulation of transcription in breast cancer tumorigenesis.

In the METZ LAB ...



Metz group 2014.

The Metz group continues to try to understand structure and bonding in gas-phase metal ion complexes and to explore their photodissociation dynamics. Graduate student **Abdulkadir Kocak** is studying how binding to transition metal ions weakens the C-H bonds in methane, the initial step in C-H bond activation, by measuring vibrational spectra of $M^+(CH_4)_n$ complexes. He has extended his measurements of cobalt and nickel complexes, done

with Zach Sallese (BS '13), to those of copper and silver. Muhammad Affawn Ashraf, a first-year graduate student, worked on these studies and is extending them to C-H activation by metal cluster ions, a focus of our new NSF grant. Postdoc Wright Lee Pearson and graduate student Chris Copeland completed their studies of the electronic spectra of Mn⁺-water complexes. By analyzing the vibrational and rotational structure in the spectrum, they determine how the electronic configuration of the metal affects the vibrational frequencies, M*-water bond strength and geometry of the complex. Wright, graduate student Dave Johnston and undergraduates Richard Dusablon (BS '13) and Annikki Santala are optimizing our photofragment imaging instrument to measure photodissociation dynamics of ions. This instrument measures the amount and direction of the kinetic energy released when ions photodissociate. This allows us to measure bond strengths and reveal information on short-lived excited electronic states.

In the ROTELLO LAB ...



Rotello group 2013.

2013 featured comings, goings and much happening in the Rotello Lab. Vince Rotello was appointed Editor in Chief of Bioconjugate Chemistry, and is currently getting social media up and running at the journal while handling the incoming manuscripts. Group members won three prizes in the ResearchFest 2013: Congratulations to Daniel, Krish and Ryan! Vince was among the recipients of the CVIP Technology Development award. On the departure side, Xi Yu, Subinoy Rana and Chandra received their PhDs, with Xi heading to Tel Aviv, Subinoy off to Imperial College in London and Chandra direct to Intel. On the incoming side, Akash Gupta, Joseph Hardie, Riddha Das and Yuanchang Liu have officially joined our group. Joseph Hardie is a joint student of Profs. Rotello and Farkas. Publications continued apace, with 23 in 2013. These publications are making an impact, with over 2500 citations last year, and Vince hitting an h of 70. Industrial collaboration featured strongly in the group, with funding from Ferminich and Teijin. New Federal funding included \$280K from the National Academies for test strip sensing of drinking water purity and \$400K from the National Science Foundation for development of nanoplasmonic sensors.

For up-to-date news, please check out http://www.umass.edu/rotellogroup/ or see what's up on our less formal Facebook page https://www.facebook.com/rotellogroup.

In the SCHNARR LAB ...

The Schnarr lab continued to explore the biosynthesis of drug-like small molecules in soil bacteria. After four long years of hard work, Tsung-Yi Lin successfully cloned and characterized the biosynthetic cluster responsible for production of fluvirucin B1. This unique metabolite provides a new avenue toward the discovery of improved antibiotics and may hold the key to a better understanding of the evolutionary relationship between fatty acid biosynthesis and polyketide biosynthesis. This work was published in ACS Synthetic Biology late last year and has garnered much attention from the research community leading to several exciting new research collaborations. Tsung-Yi is now examining the substrate selectivities of several critical enzymes within the fluvirucin biosynthetic assembly to better assess the engineering possibilities for this system.

In other news, 2013 marked the end of an era in the Schnarr lab. The original three graduate students brave enough to join a budding young research program have now moved on to next phase of their careers. Gitanjeli Prasad was the first to successfully defend her thesis involving the development of small molecule probes for analyzing biosynthetic enzymes. Soon after, she moved to her current position as a postdoctoral associate at Boston Biomedical. Jon Amoroso and Lawrence Borketey followed suit just a few months later. Jon has recently accepted a teaching position at the College of the Holy Cross and Lawrence has moved back to Ghana to be with his new bride and seek a position in academics. The remaining Schnarr lab members wish these pioneers the best of luck in their current and future endeavors.

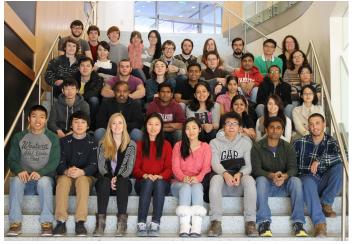
And last but certainly not least, after a grueling couple of years, Adam Gann has successfully developed a photoinduced, copper-free click reaction. This high-yielding process is complete in just minutes and relies on a reactive benzyne intermediate formed from photolysis of a triazenebenzoic acid precursor. The reaction shows great promise for site-specific labeling of dynamic systems that require precise spatiotemporal control. Adam's work was recently submitted for publication and with any luck should be coming soon to a journal near you.

In the THAYUMANAVAN LAB ...

The Thayumanavan group enjoyed another productive year in 2013. Please visit our new and renewed website at https://elements.chem.umass.edu/thaigroup/ for more on our news and achievements (thank you Lisa for the help in setting this up). Also follow our group on Facebook or Twitter (links

provided in our website). If you are a group alum and we do not have your updated whereabouts, please let us know. Below, we are listing a few of the people highlights from the group.

Graduate students update: The group welcomed Mina Canakci, Bin Liu, Uma Sridhar, Dongsik Yang, and Bo Zhao. Mina is a joint student with Barbara Osborne and Lisa Minter (Veterinary and Animal Sciences) and Bo is a joint student with Richard Vachet. Molly Gordon has been selected for a two-year fellowship through the NIH-sponsored Chemistry-Biology Interface (CBI) Training Program. Jiaming Zhuang was awarded the prestigious graduate school fellowship award for this year. Judy Ventura completed a summer internship at the Boehringer Ingelheim Pharmaceuticals in the Analytical Development Department. Andrea Della Pelle finished her PhD recently and has taken a job as Scientist at Brewer Science in Missouri. Feng Wang finished her PhD and started as Scientist at the Sid Richardson Company in Dallas. Diego Amado Torres will soon graduate and join Bosch in California. Last year, Jack was just leaving to pursue entrepreneurial opportunities, he is doing that now. Jack is now an Investor Analyst at Life Science Nation in Boston. Daniella Gonzalez has been already promoted in her company, L'Oreal. Our alum Conghui Yuan has been appointed as an Associate Professor at the College of Materials in Xiamen University.



Thai group 2013.

Undergraduate students update: Louis Pires and Paul Yao have graduated. Will White spent his summer doing an REU in Southern Mississippi. Brendan Abbott, Kevin Byrne and Garrett Loomis joined our group for their undergraduate research recently. Arda Kotikian, a student in Mount Holyoke College, worked as an undergraduate researcher in our lab over the summer.

Postdoctoral associates and visitors update: Mijanur Molla joined the group as a postdoctoral associate.

Subrahmanyam (Subbu) moved to McMaster University in Canada as a postdoctoral associate. The group welcomed Cunfeng Song and Yiting Xu as visiting graduate student and visiting faculty respectively; they are both from Xiamen University. Sivakumar Aathimanikandan and KN Jayakumar moved to new jobs in Indiana and Massachusetts, respectively. R. Prakash Babu is now a postdoctoral fellow at KAUST in Saudi Arabia. Jaggavarapu Sreedhar Reddy has a new position at SABIC in Bangalore.

Thai had the opportunity to interact with alums during two of his international trips. Xinlin Yang, who was our alum and now an Associate Professor at Nankai University, accompanied him throughout his trip in China for a week attending conferences and giving talks at various places in China. Thai also co-organized an Indo-US workshop in Thiruvananthapuram, India. Besides listening to great science including from three of the Thai group alums (Ashootosh, Krishnamoorthy, and Suhrit), the highlight was that the workshop was co-organized with Suhrit Ghosh. Finally, Thai was also recognized at the UMass Faculty Convocation with an Award for Outstanding Accomplishments in Research and Creativity.

In the **THOMPSON LAB** ...

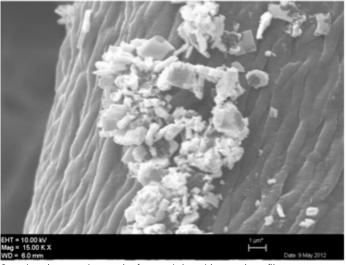
It's been a busy year in the Thompson Lab! Prof. Thompson spent January-July on sabbatical at Caltech, where she initiated an electron cryotomography collaboration with Ariane Briegel and Grant Jensen. The beautiful images that we obtained show that our functional complexes of chemoreceptor proteins (made either with molecular crowding agents or with Bob Weis' templating vesicle technology) are forming large hexagonal arrays that are much more native-like than other in vitro preparations being studied elsewhere!

Meanwhile, back at UMass, the group worked hard to move into a new beautiful laboratory, shared with the groups of Min Chen and Craig Martin. This 8th floor laboratory is enhancing research productivity and promoting sharing of ideas and expertise among these groups and also with our new neighbors in the 7th floor shared labs of Matt Holden, Jeanne Hardy, and Michelle Farkas. Lynmarie was thrilled to see the group working happily in the new lab when she visited from Caltech in April for Seena Koshy's successful PhD defense. The summer brought more great news: with the state investing \$95 million in life sciences research at UMass Amherst, a complete upgrade of the NMR facility is now in progress, with the purchase of four spectrometers, including a 600 MHz solid-state instrument! This will be of tremendous benefit to our research, as we continue to investigate the transmembrane signaling mechanism of chemotaxis receptors, using a combination of biochemical methods to assemble and characterize functional complexes, a new hydrogen exchange mass spectrometry approach to probe dynamics, and solid-state NMR to probe structure in these amazing signaling arrays.

Unfortunately, this year also brought the tragic loss of our colleague and collaborator **Bob Weis** in October. The sheer number of people who came to pay their respects was a testament to the many lives he touched. In spite of the sadness of the occasion, it was nice to reconnect by phone or email or in person with many alumni of the **Weis** and Thompson and **Martin** labs.

In the TYSON LAB ...

In the Tyson lab, in the spring semester, undergraduates Jill Carlson and Polina Berdnikova worked alongside doctoral student Nan Wang and a visiting scientist from Brazil, Dr. Aline Silva. Polina developed a modification to the t-test for use with standard reference materials. Jill and Aline obtained our first data on the inhomogeneity of the arsenic concentrations in bags of rice, while Nan and Aline continued the hunt for the elusive volatile arsenic compound that is lost when rice is oven dried. Aline returned to Brazil at the end of the summer and is planning further post-doctoral work and eventually a faculty position. We were again involved with the STEM DIGITAL summer workshop for K-12 teachers. Digital Images in Geoscience Investigations: Teaching Analysis with Light is an NSF-funded program enabling high school and middle school teachers and students to conduct environmental research aided by the analysis of images from digital cameras, scanners, and the Internet (see http:// k12s.phast.umass.edu/digital/). Materials developed for the workshops were repurposed for an online course in the fall taken by in-service teachers in the Science Education Online master's degree program (http://www.umass.edu/seo/). Arsenic in the environment was packaged as two, one-week modules. Also in the fall, three undergraduate participants the College of Natural Sciences First-year Research Experience, worked on arsenic-related topics. In this program, well-qualified incoming first-year students work in a faculty member's research group in their first semester. The program has been running for four years now and has grown to accommodate over 40 students (see https://www.cns.umass.edu/about/eventphoto-galleries/12-23-2013/first-year-research-experienceposter-session-2013). Lauren Okamoto and Harry Lu worked on the continued development of a "kitchen" procedure for the determination of arsenic compounds in rice, and Daniel Piersiak worked with Nan to study the concentration of arsenic in individual rice grains, which appears to be much less uniform than we thought. Nan successfully defended her dissertation in December 2013. This brings the total of "Tyson doctoral students" to 52 and closes the set. Her work on inorganic arsenic speciation in waters by a method based on selective hydride formation reaction chemistry and atomic fluorescence spectrometry will appear shortly in the Journal of Analytical Atomic Spectrometry. The arsenic project that involves groups of undergraduates, mainly from the CHEM 121H and 122H, in authentic research has been redesigned and now takes place on one afternoon each week in the



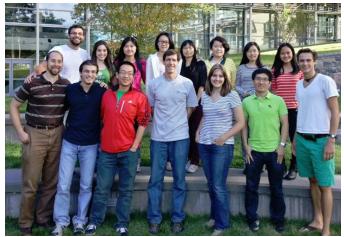
Scanning electron micrograph of mercuric bromide crystals on filter paper exposed to arsine gas. Chengbei Li's research into the thermodynamics of the Gutzeit modification of the Marsh test for arsenic.

3rd floor analytical/physical teaching lab in the Integrated Sciences Building. About 30 students participated in the spring, and 18 students in the fall. The fall "class" was helped considerably by a former graduate student Dr. Hans Mentzen (who is currently teaching general chemistry), and a former undergraduate researcher, Bill Rowley, who is currently a member of the UMASS postbaccalaureate research education program, PREP, (http://www.umass.edu/prep/). A new aspect of the arsenic project is underway, in which high school students (taught by Andrew Patari at the Four Rivers Charter School in Greenfield) are also working on topics related to the measurement of arsenic in rice. Prof. Tyson is also breaking new ground teaching CHEM 101 as an online course, though neither of the two offerings so far has been either massive or open. This is a general education course for non-science majors, subtitled "How Much Arsenic Do We Eat?" Profs. Peter Uden (emeritus), and Ed Voigtman, continued to make welcome inputs to group activities. Prof. Tyson can be found on LinkedIn.com.

In the VACHET LAB ...

Research in Vachet group continued in the areas of amyloid fibril formation of $\beta\text{-}2\text{-microglobulin}$ and new mass spectrometric tools for detecting nanoparticles in cells and tissues. With a new grant from the NIH, we have also recently ramped up our collaboration with Prof. Thayumanavan's group and are now exploring the use of his group's amphiphilic homopolymers for the enhanced detection of biomarkers by mass spectrometry. We published seven papers in 2013, including several papers in Analytical Chemistry and the Journal of the American Chemical Society. Prof. Vachet and group members also made 20 presentations at various conferences, meetings, and universities.

In other group news, we were sad to say good-bye to Jia Dong, Adam Graichen, Feng Wang, and Yuping Zhou. Feng, Jia,



Vachet group 2013

and **Yuping** all successfully defended their PhDs within a 10-day span in September, just before Prof. Vachet's three month sabbatical in Germany. **Feng** left to work at Sid Richardson Carbon and Energy Company in Texas; **Jia** headed to Shire Pharmaceuticals for a postdoctoral position; and **Yuping** is now at Eli Lilly in Indianapolis. After seven years as a grad student and postdoc in the lab, **Adam** also departed to take a job at Excellims in Acton, MA. Our mass spectrometers will never be the same without **Adam**'s uncanny ability to fix and maintain them.

We also welcomed two new members to the lab—Singyuk Hou, who is co-advised by Vince Rotello, and Mahalia "Mac" Serrano. Singyuk is working to make nanoparticles more detectable in tissues, and Mac is using amphiphilic polymers and mass spectrometry to make biomarkers easier to measure in serum.

In alumni news, former graduate student Jiang Zhu will soon begin his faculty position at the Interdisciplinary Research Center for Biology and Chemistry (IRCBC) at the Chinese Academy of Sciences. He and his wife were also blessed with a baby girl (Angela) in May. In more baby news, former graduate student Vanessa Gill and her husband celebrated the birth of Alex, and former graduate student Jon Wilson and his wife welcomed baby James. Finally, former graduate student Matt

Miller was recently promoted to a CMC Project Manager position at Forest Laboratories in PA. He also played a big role in the drug LinzessTM, which was released recently.

Finally, Prof. Vachet was very busy professionally. He served on the Editorial Board for the *Journal of the American Society for Mass Spectrometry* and the Features Panel for *Analytical Chemistry*. He also served as Vice-Chair of a Gordon Conference in July and is in the final stages of planning a Mass Spectrometry meeting in Florida.

In the VENKATARAMAN LAB ...

Follow the DV group on Twitter at **dvgroupumass** or go to to their website at **thedvgroup.com** for the latest news and updates.

In the VOIGTMAN LAB ...

For the first eight months of 2013, I served as associate head, undergraduate program director and acting graduate program director. Then, on the first of September, I became plain old associate professor and I have to say it is great being a nobody! I taught CHEM 111 both spring and fall semesters, and used CTFD funding to upgrade my iPad teaching technology. I also did research with two undergraduates (Jill Carlson and Artur Wysoczanski) and we have a paper currently under review.

Uma Kale (PhD with me), who is married to Ebenezer Debrah (PhD with Julian Tyson), sent along a photo of their beautiful daughter Anjali, who is growing up fast! I got see Dan Montville and his wife Lauren at Elena Dodova's Memorial service on September 14th. They are both doing well and like their jobs. Richmond Ampiah-Bonney and Angela Fahey did a terrific job making the Memorial service happen. Elena was very special in many unexpected ways and we miss her wide-eyed "but, anyway, it's a big chaos" take on life. We also lost Prof. Bob Weis in October. More about it on page 21.

My sabbatical leave starts January 19, 2014, and I have already finished several chapters of the book I am writing on limits of detection. I will be retiring in summer, 2015, so best of success to all and please stay in touch!

dissertation DEFENSE SEMINARS

GRADUATE STUDENT	SEMINAR TITLE	DATE	PI
Nitai Charan Giri	"Structural Investigations of Early Catalytic Intermediates and Nickel Inhibition Complexes of Human DNA and Histone Demethylases"	January 30, 2013	Michael J. Maroney
Bhooshan C. Popere	"BODIPY-Based Panchromatic π-Conjugated Polymers for Organic Photovoltaics"	February 8, 2013	S. Thayumanavan

GRADUATE			
STUDENT	SEMINAR TITLE	DATE	PI
Reuben Thomas Chacko	"Design and Development of Nanogels for Small Molecule and siRNA Delivery"	March 5, 2013	S. Thayumanavan
Kelly Cathleen Ryan	"Investigation of the Structure/Function Relation- ship in Nickel Containing Superoxide Dismutase"	April 8, 2013	Michael J. Maroney
Seena Smitha Koshy	"Differences Between Bacterial Chemotaxis Receptor Signaling States Revealed by a Novel Hydrogen Exchange Mass Spectrometry Approach"	April 9, 2013	Lynmarie K Thompson
Handan Akpinar	"Molecular Crystal Assembly of Organic Radicals and Biradicals"	May 8, 2013	Paul M. Lahti
Guanbo Wang	"Tools for Probing Protein Higher-Order Structure: Monitoring Aggregation with Native ESI-MS and Conformational Dynamics with Top-Down H/D Exchange MS"	May 9, 2013	Igor A. Kaltashov
Gitanjeli Prasad	"Reactive Heterocycles for Examining Polyketide Biosynthesis"	May 20, 2013	Nathan A. Schnarr
Shunhai Wang	"Development of Mass Spectrometry-Based Methods for Quantitation and Characterization of Protein Drugs: Transferrin as a Model Drug Delivery Vehicle"	May 23, 2013	Igor A. Kaltashov
Max Lein	"Droplet-Interface Bilayer Technologies for Membrane Protein Analysis and Molecular Trafficking Measurements"	June 4, 2013	Matthew Holden
Sravan K. Surampudi	"Conjugated Molecules and Materials as Viable Platforms to Study Light-Matter Interactions"	July 8, 2013	D. Venkataraman
Serap Pektas	"O ₂ Activation and Allosteric Zn(II) Binding on HIF-Prolyl Hydroxylase-2 (PHD2)"	August 8, 2013	Michael J. Knapp
Sheringham Lawrence Borketey	"New Tools for Probing Polyketide Biosynthesis"	August 23, 2013	Nathan Schnarr
Jacob A. Harvey	"Clustering, Reorientation Dynamics, and Proton Transfer in Glassy Oligomeric Solids"	August 28, 2013	Scott M. Auerbach
Andrea M. Della Pelle	"Design and Syntheses of Donor-Acceptor Dyads and Triads for Improved Light Harvesting in Organic Photovoltaics"	August 28, 2013	S. Thayumanavan
Jon Amoroso	"Reactive Probes for Manipulating Polyketide Synthases, and Photoreactive Probes for Strained Alkyne Click Chemistry"	August 30, 2013	Nathan Schnarr
Feng Wang	"Amphiphilic Supramolecular Assemblies and Their Applications in Materials and Biology"	September 16, 2013	S. Thayumanavan & Richard Vachet
Jia Dong	"Mass Spectrometric Methods for Studying Protein-Metal Binding"	September 23, 2013	Richard W. Vachet
Ebru Kizilay	"Coacervation of Oppositely Charged Macromolecules, Micelles and Proteins: Disproportionation and Hierarchical Structures"	September 24, 2013	Paul L. Dubin
Yuping Zhou	"Structural Analysis of Proteins by Covalent Labeling and Mass Spectrometric Detection"	September 26, 2013	Richard Vachet
Muslum Yildiz	"Allosteric Regulation of Dengue Virus Type-2 Protease"	October 24, 2013	Jeanne A. Hardy



Jake Pawlowski and Cedric Bobst (Kaltashov group)

with state-of-the-art instrumentation for biophysical characterization, mass spectrometry, optical microscopy, and more, will be created. These facilities and others on campus are being equipped and enhanced using the MLSC funds. For example, the NMR facility will have a total upgrade and replace aging instruments with new Bruker spectrometers operating at 500 and 600 MHz.

The IALS central mission is to enhance the translational applications of our top-notch life sciences research programs on campus, including formation of new partnerships with industries, especially in the Commonwealth. In addition, the establishment of IALS will better fulfill the campus training and education goals, helping to better prepare our students to join the workforce of the Commonwealth and beyond. Within IALS, there are three Centers: Models to Medicine (M2M), Bioactive Delivery (CBD), and Personalized Health Monitoring (PHM). The spectrum of research focuses of these centers spans molecular structure, disease target identification, and small molecule discovery for potential therapeutic targets (M2M); delivery of drugs including targeting to specific tissues and cell types (CBD); and design of devices to make measurements of health-related parameters (PHM). To learn more about IALS and the centers, go to www.umass.edu/ials.



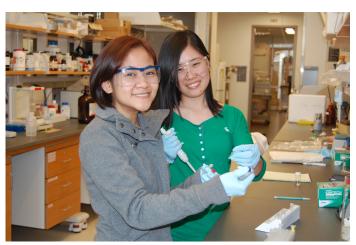
M2M is hosting a kick-off symposium on "Models to Medicine: Challenges and Opportunities," Friday, May 2, 2014. Go to www.umass.edu/m2msymposium/ for details of this event.

The impact of the MLSC funding and the new building are being felt already!!! New industrial partnerships have been formed, synergistic research collaborations are being created, and plans for faculty hiring are being coordinated in interdisciplinary ways.

INTERVIEW WITH PROFESSOR RICHARD VACHET (RV)

GG: How will the new facilities in the Life Sciences Laboratories enhance your collaborations and foster new ones? Has it done so already?

RV: The new facilities have enhanced my emerging collaboration with Peter Chien from BMB. Because now my students and his students are on the same floor, we don't have to go far to transfer samples, talk about results, or plan the next set of experiments. Peter and I also now have offices just down the hall from one another, so we don't have to go out of our way to meet. We have a lot more informal meetings.



Mahalia Adelina Corazon Serrano and Meizhe Wang (Vachet group)

Graduate students in my group are also now seeing and interacting with new people with similar research interests. This has led to some nice "cross-talk" that will likely lead to them better doing their own experiments and coming up with new research ideas. Graduate students are also learning about all the other tools that are available to them as they interact more closely and effectively with students from other groups. That means we are able to help some students from other groups with, say, mass spectrometry measurements, and other groups have been able to help us with tools we don't already have in our lab.

In addition to the new Life Sciences Lab, several Chemistry groups are in recently renovated space in Lederle. These NIH-funded renovations were featured in last year's

STATE OF THE ART LABORATORIES—continued from page 16



Jing Huang (Holden group)

Goessmann Gazette. Now that they've been in the new space for a year, Professors Holden, Hardy and Rotello reflect on how the upgraded facilities have affected their research.

INTERVIEW WITH PROFESSOR MATT HOLDEN (MH)

GG: How do you think the open floor plan in the newly renovated LGRT 7th floor labs will affect your research, and what advantages do you foresee?

MH: The key aspect of the floor plan for our lab is the custom engineered electrophysiology suite. Here, our fluorescence microcope and electrical recording equipment are totally isolated from the outside world, allowing for better signal to noise ratios than in conventional laboratory space. With this advance, we predict that we may be able to probe our systems more sensitively than ever before.

GG: How does your new lab foster collaborations, and if so, how do you see this happening?

MH: Luckily for us, we share the lab floor with Professors Hardy and Farkas who bring a wealth of biochemical and cell biology expertise right next door to our lab. This will be extremely useful as a source of information and ideas as we pursue our research in model membrane systems. In addition, our lab possesses unique microfabrication capabilities that will be of great utility to others on the floor. We can custom design virtually any type of plastic device with our equipment, which we frequently use in our experiments.

GG: What is your favorite new lab feature? **MH:** The space is clean, sleek and open. The lab was essentially designed around the specific needs of our experiments, so every piece of equipment sits in its own niche with the necessary accessories and facilities within easy reach. This has really sped up our experimental routine.

GG: What are your students liking most about the new lab? MH: My students really appreciate the close proximity to the other labs. Mainly, the custom electrophysiolgy room is the feature everyone likes the most since the environment has been tailored to suit our needs.

GG: What new instrumentation are you able to operate in your new lab?

MH: Due to the noise isolation, we can now couple fluorescence and electrical measurements synchronously which we were not able to do before.

GG: How does your new lab allow you to compete with researchers at other universities?

MH: With the enhanced capabilities afforded by the new space, we will enter into research areas and pursue exciting fundamental questions that might not be accessible at other facilities, providing us with a key advantage for future endeavors.

UPDATES FROM THE HARDY AND ROTELLO LABS

During her initial years at UMass, the Hardy lab was very tightly packed into a small amount of lab space, waiting for planned renovations. We bought everything in miniature. The most amazing aspect our our new labs are that we now have space to work "full-sized." This has pleasantly impacted how many people can, for example, purify proteins simultaneously. We are thrilled that the new space was also designed to enable us to open a tissue culture facility that we share with a new faculty member on the floor, Michelle Farkas. This tissue culture facility allows us to assess how our caspase reporters work and test our caspase-6 inhibitors for the efficacy in an Alzheimer's context. This is our first time to be near so many other chemistry colleagues. This proximity has lead to captivating new interactions and collaborations.

The renovated labs on the 3rd floor for the Rotello group have been hugely successful in fostering a collaborative work environment. The open floor plan mixes chemists, biologists and materials scientists, while the library and break/lunch room provide informal places for people to discuss research and socialize. There have been a few changes in how we use the space compared to the original plan. The most obvious change has come from our move into sensing pathogenic bacteria, which caused us to make our materials processing room dual-purpose. This required the materials folks to take a biosafety course, eliciting some quiet grumbling but providing more broadly trained materials scientists!

iCons reaches several milestones

On January 18, 2011, iCons Program Director Scott Auerbach observed from the back of a lecture hall in UMass Amherst's Integrated Sciences Building as the first cohort of iCons scholars – known affectionately as "the guinea pigs" – brought the first iCons course to life.

"Standing in that room and listening to these students, I realized in the deepest part of my heart and mind that we were on the right track," he said. "It was better than we ever could have hoped."

What Auerbach and his team hoped for is captured in the program's mission: To produce the next generation of leaders in science and technology with the attitudes, knowledge, and skills needed to solve the inherently multi-faceted problems facing our world.

FROM GUINEA PIGS TO GRADUATES

Now with the guinea pigs entering their fourth and final semester, the first full cohort of iCons scholars will soon head into the real world to realize this mission. When these students graduate in May, the program will reach an important milestone as well. From an idea proposed in 2006, iCons has evolved into a living, breathing, four-year academic program that is uprooting expectations about what undergraduates are capable of achieving.

iCons is not just a class, it's an attitude for approaching the world."

More than just maturing, iCons is thriving. The number of applicants has grown each year, and the increasing interest has helped fulfill one of the primary goals of the program – integration between disciplines. In the first year, the applicants represented 10 majors in two colleges. This year's pool of applicants encompassed 25 majors and five colleges.

The growth is due in large part to the program's most vocal advocates: its students.

AN ATTITUDE FOR APPROACHING THE WORLD

"iCons is not just a class, it's an attitude for approaching the world," explained Debbie Tschong, a junior and member of the second iCons cohort.

Embodying the philosophy that in iCons, nothing is "just a classroom exercise," Tschong and fellow students Erin Amato and LeAnn Monteverde were inspired to bring the program's team-based approach to problem solving into the real world. Last fall, the students helped organize and lead iCons case study workshops with participants in Girls Inc., a program that provides academic support and mentorship to girls from underserved communities.

The initiative has blossomed into a partnership with UMass Civic Engagement and Service Learning, which will establish two internships exclusively for iCons students to work with Girls Inc. over the summer. It's an indication of the program's level of commitment to training the next generation of science leaders, not only by raising the bar in STEM education at UMass, but by reaching out to help level the playing field so students of all backgrounds can succeed.

TRAILBLAZING NEW PARTNERSHIPS: WATERS CORPORATION

The iCons Program reached another critical milestone last year – securing its first corporate sponsor: Waters Corporation of Milford, MA, an analytical services company with over a billion dollars in annual revenues. Dan McCormick, the chief technology officer for Waters was so excited when he first learned about iCons, he said "this is something that Waters has to be a part of, for our own self-interest to hire iCons interns and graduates, and also to help shape the future of technology education."

Indeed, the relationship between iCons and Waters is doing exactly that – trailblazing a new partnership model between industry and academia. The problem-based iCons teaching model opens the possibility of bringing real-world industry problems into the iCons classroom. Dr. McCormick jumped at the opportunity to bring Waters problems into the iCons classroom. Doing so required a new legal contract – an "educational cooperation agreement" – allowing iCons faculty access to Waters intellectual property (IP).

"Jumping into this partnership required leaps of faith on both sides," said Chemistry professor and iCons Program Director Scott Auerbach. "Waters had to believe their IP will remain safe, and we in iCons had to believe that our classes will remain totally in our control. During all our conversations, there was never a doubt that this partnership is a win-win."

We cannot wait to see how the Waters-iCons case study turns out. Please stay tuned for next year's issue of the Goessmann Gazette to find out.

To learn more about the iCons program, please visit our website: www.cns.umass.edu/icons-program.



2013 SEMINAR SERIES

Continuing the long-standing tradition, the 2013 UMass Amherst Department of Chemistry seminar series has drawn many outstanding scientists to our campus to share their insights and recent developments. Some of the highlights included seminars from several distinguished speakers.



Professors Jane Rausch and Jerry Atwood

Professor Jerry Atwood from University of Missouri-Columbia was our *Marvin D. Rausch Lecturer in Organometallic Chemistry* this year. Prof. Atwood is a world known leader in the field of supramolecular chemistry. He has authored over 690 publications in refereed journals, and 20 book chapters, and also holds 13 patents. On March 28, he gave a talk entitled "Metal-Organic Nanocapsules for Targeted Drug Delivery." In his talk, he described a fascinating approach of using macrocycles, e.g pyrogallol[4]arenes to form nanocapsules as carriers to courier drug molecules across the cell membrane.

Each year the UMass Amherst and Smith, Mt. Holyoke, Amherst and Hampshire Colleges co-host the *5-College Lecture Series in Chemistry*. For 2013, we were delighted to have **Prof. Geoffrey W. Coates** from Cornell University to be our speaker. In 2011 he was identified by **Thomson Reuters** as one of the world's top 100 chemists on the basis of the impact of his scientific research, and was inducted into the American Academy of Arts & Sciences. He received the Presidential Green Chemistry

Challenge Award and the DSM Performance Materials Award in 2012. In his seminar "New Polymers from Old Monomers: Advances Enabled through Catalyst Design and Discovery" he presented the discovery, development and application of new catalysts for synthesis of inexpensive new polymers.

Professor Christopher Ober from Cornell University gave the *Stein-Bayer Honorary Seminar in Polymer Chemistry* on October 3. **Prof. Ober** is a Francis Bard Professor of Materials Engineering and a leading expert in the polymer science. He is well known for his pioneer work on new materials for photolithography and studies the biology materials interface. His awards include the 2013 SPSJ International Award, 2009 Gutenberg Research Award from the University of Mainz, the 1st Annual FLEXI Award in the Education Category (for flexible electronics) awarded in 2009, a



Professors Min Chen, Geoffrey Coates, Dhandapani Venkataraman



Professors Christopher Ober and Richard Stein

Humboldt Research Prize in 2007 and the 2006 ACS Award in Applied Polymer Science. **Prof. Ober** presented a lecture entitled "Polymer Brushes: Patternable structures as interfaces with the biological environment." In this talk, he described several polymer brush systems to control interaction of biomacromolecules and cells by design of specific and non-specific interactions.

On October 10, the 2013 *William E. Mahoney Annual Lecture* was given by Prof. Peter Schultz from the Scripps Research Institute. Prof. Schultz is well recognized for his pioneer work on developing methods that include new building blocks beyond the 20 common amino acids to expand the genetic codes of living organisms. He founded and was the Institute Director of the Genomics Institute of the Novartis Research Foundation (GNF) in San Diego, CA from 1999 to 2010 and more recently (2012) the California Institute for Biomedical Research (CALIBR), a not-for-profit institute focused on early stage translational research. In addition, Schultz is a founder of Affymax Research Institute, Syrrx, Kalypsys, Phenomix,

Symyx Therapeutics, Ilypsa, Ambrx, Ardelyx, and Wildcat Technologies, pioneers in the application of diversity based approaches to problems in chemistry, materials science and medicine. His lecture, "Synthesis at the Interface of Chemistry and Biology: From Stem Cells to the Genetic Code" described how his group combined the tools and principles of chemistry

with the molecules and processes of living cells to synthesize novel molecules and molecular assemblies with novel physical, chemical and biological functions. Examples of this synergistic chemical/biological approach to synthesis included the addition of unnatural amino acids to the genetic codes of prokaryotic and eukaryotic organisms, and the identification of small molecules that control stem cell self-renewal and directed differentiation, as well as reprogramming of somatic cells.

We are grateful for the generous contributions of our alumni and corporate sponsors, who make the success of the seminar program possible. More information about the upcoming seminars and events can be found at www. chem.umass.edu/events/. We look forward to another exciting seminar series in the next year!



Robert Mahoney and Prof. Peter Schultz

inMEMORIUM



We are deeply saddened by the passing of our colleague, **Professor Bob Weis**, on Sunday, October 20, 2013 following a long battle with cancer. Bob was a wonderful colleague, scientist, teacher, mentor, and friend, who will be missed by many. He joined the department in 1988 as the first hire of a departmental expansion into biological chemistry. The focus of Bob's research was to understand biological membranes and membrane proteins, by strategically combining biochemical tools with careful spectroscopic and thermodynamic measurements. He and his group made many contributions to understanding the signaling mechanisms of bacterial chemotaxis receptors, which enable bacteria to "smell" their environment and direct their swimming behavior. Such fundamental sensing and signaling processes enable communication between cells of multicellular organisms for the coordinated actions that make life possible. During the course of these studies, Bob and

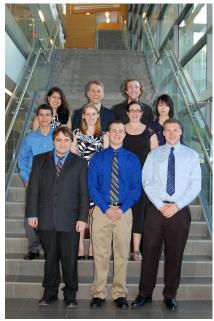
his group developed a a novel approach for bypassing some of the challenges of working with membrane proteins, by binding a soluble fragment of the receptor to vesicles to restore its activity. Since many drug targets are membrane proteins, Bob recognized the potential of this methodology for drug screening and co-founded a company, Protein Attachment Technologies, to further develop it. Bob's careful and insightful science has had significant impact: a number of his



publications have been cited over 100 times, with a total of about 2000 citations by other articles thus far. Bob loved doing science, and he shared that science with numerous graduate students and undergraduates who trained in his laboratory. He touched many lives, and we will miss his insights and his wry humor.

Paul H. Terry, 85, of Beltsville Maryland (formerly of Assonet, Massachusetts) passed away on Monday November 18, 2013. He was born in Fall River, the son of the late Job H. and Mabel (Burns) Terry. He graduated from Dighton High School class of 1946 and Bradford Durfee Tech with a bachelor's of science degree in 1951. Paul earned a Master's degree in Chemistry in 1959, and received a PhD in Chemistry in 1963 from his work with Professor Louis Carpino. He served his country during the Korean War with the United States Army. Dr. Terry worked for the United States Government as a research chemist before retiring many years ago. He was a member of the American Chemical Society, American Institute of Chemists, past president, councilor and board manager of Greater Washington Institute of Chemists, and the Toastmaster's International. Paul was very active and enjoyed the time he spent with his family and friends over the years. He is survived by an aunt and several cousins and good friends. Dr. Terry was a dear friend and devoted supporter of the Department of Chemistry; he fondly recalled his past here, and was enthusiastic about the future of Chemistry as well, and he will be missed.

undergraduate SENIOR & AWARDS DINNER



The 2013 Senior Class.

Every May, as is our tradition, at our annual Undergraduate Honors and Awards banquet we honor students who have proven themselves to be among the very best this University has to offer. During the spring, the Undergraduate Honors and **Awards Committee** had the pleasure of examining the records of students who had chosen to be

a part of our department in order to determine who shall be recognized for their achievements. Last spring we recognized the hard work and dedication of 32 graduating seniors. In addition, many students were recognized for their work within the department: see the complete awards list. These awards are only possible because of the generous support the department receives from our alumni, industrial partners and professional organizations. With considerable pride and gratitude, the committee wishes to thank our outstanding students for their contributions to the department and university and wishes to thank those who, in turn, support our students.

The following students received awards:

Rebecca C. Bishop—Connecticut Valley Section of the American Chemical Society (CVS/ACS) Student Award **Deborah J. Ehrlich**—American Institute of Chemists Award

Michael T. Veling and Jeffrey Boerth-Richard W. Fessenden Award

Melanie P. Muller-John A. Chandler Memorial Scholarship Award

Katherine Y. Williams-Duhamel and Zachary W. Sallese –Merck Index Award

Felix S. Alfonso and Kathryn M. Liedell-Senior Class Award

Felix S. Alfonso-Hypercube Scholar Award Stan Najmr-ACS Inorganic Chemistry Award Kathryn M. Liedell and Melanie P. Muller -Departmental Recognition Award

Kathryn M. Liedell, Meaghan A. Valliere and Di Lin
–Uche Anyanwu Memorial Award for Outstanding
Research 2013

Artur Wysoczanski-ACS Analytical Chemistry Award Felix S. Alfonso-Jay A. Pirog Scholarship Meaghan A. Valliere-Bradspies Research Fellowship Kathleen A. Dreher-Bates Research Fellowship Nicholas J. Sargent and Abigail R. Sossen-American Chemical Society-Hach Fellowship

Di Lin, Katherine Y. Williams-Duhamel, Molly A. Cocaine, Katie L. Callahan and Shera A. Demchak –Edward Shapiro Scholarship

Jeffrey F. Goulette-Mr. Tompkins Award Shera A. Demchak-Oliver Zajicek Memorial Scholarship Award

Laurel L. Banach, Nicole M. Gullotti and Sasha L. Santiago-Robert Maxwell Williams Memorial Scholarships

Jonathan T. Dullea, Kate V. Daborowski, Julianna E. Tordella and Steven R. Ayotte-CRC Freshman Chemistry Award

degrees AWARDED

BA/BS DEGREES Zachary G. Hitzig 02/2013 09/2012 Felix S. Alfonso 05/2013 Joseph R. Perito Kelvin S. Laurore 05/2013 Louis A. Pires 05/2013 Denis Ashlaban 05/2013 05/2013 Gina M. Lein Zachary W. Sallese Rebecca C. Bishop 05/2013 Kathryn M. Liedell 05/2013 Denis, I. Shlosman 02/2013 leffrey Boerth 05/2013 Justin A. Srodulski Jillian R. Carlson 05/2013 05/2013 05/2013 Jennifer K. Ludwig Michael T. Veling (dual major) 05/2013 Avery A. Compton 05/2013 Philip T. McGilvray 05/2013 Austin J. Virtue 05/2013 Shera A. Demchak 05/2013 Daniel A. DiCorpo 05/2013 Stan Najmr 02/2013 Katherine Y. Williams-Duhamel 05/2013 Joey M. Nguyen Penghao Yao Deborah J. Ehrlich 05/2013 Sean M. Fleuriel 02/2013 Kevin D. Olson 05/2013 M. Wengian Zhang (dual major) lacqueline L. Pasek-Allen 05/2013 Jeffrey F. Goulette 05/2013

RESEARCHFEST 2013

The Chemistry Department welcomed the 2013-2014 academic year with the 23rd annual research symposium, Researchfest. This event was held on August 27, 2013 and was a huge success thanks to the support of participants, organizers, and sponsors. The event featured four oral presentations by graduate students who were selected by a faculty committee through a nomination/evaluation



Paul Homnick, John Hangasky, Joelle Labastide, and Daniel Moyano-Marino

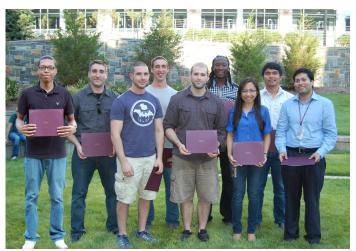
process. Joelle Labastide (Barnes Group) was chosen to receive the Richard K. and Meryl M. Brown Graduate Scholarship in Chemistry, a prize of \$5,000 for her work on "Optical Probes of the Molecular-Scale Structure of Organic Photovoltaic Materials: Investigating the Origins of Semiconducting Polymer Efficiency Limits Using Single Nanostructure Spectroscopies." Daniel Moyano-Marino (Rotello Group) received the *Dr. Paul Hatheway Terry* Graduate Scholarship Award for Outstanding Presentation for his work on "Modulating the Response of the Immune System by the Surface Engineering of Gold Nanoparticles." Paul Homnick (Lahti Group) received the *Marvin D*. Rausch Scholarship Award for Outstanding Presentation for his work on "Molecular Engineering of New Organic Electronic Materials for High-Performance Photovoltaic Devices." John Hangasky (Knapp Group) received the Marvin D. Rausch Scholarship Award for Outstanding Presentation for "Cellular O2 Sensing: Controlled O2 Activation and Reactivity by FIH."

A total of over 68 posters were presented this year. Kevin Dagbay (Hardy Group) received the 3M Award for his poster entitled, "Splicing, Prodomain, and Intersubunit Linker Impact Caspase-6 Function and Stability." The following nine students received William E. McEwen Fellowship Awards for Outstanding Posters:

- Ambata Poe (Thayumanavan Group), "Small Molecule BODIPY Dyes as Acceptors in Bulk Heterojunction Organic Photovoltaics"
- **Jeffrey Lucas** (Lahti Group), "Carpender's Rule Polymers: Simulating Folding Events Within

- Conjugated Polymers via Alkyl-Flexor Installation"
- Stephen McCarron (Chambers Group), "A Modular Kit for Traceless Labeling of Endogenous Receptors"
- Scott Eron (Hardy Group), "Allosteric Control by Phosphorylation of the Apoptotic Caspases"
- Ryan Landis (Rotello Group), "Solvatochromic Probe Detecting Hydrogen Bond Donating Solvents"
- Cornelius Taabazuing (Knapp Group), "The Gas Binding Pocket of FIH"
- Bay Serrano (Hardy Group), "Exploring Diverse Mechanisms of Regulating Caspase-9 by Phosphorylation"
- Kevin Dagbay (Hardy Group), "Splicing, Prodomain, and Intersubunit Linker Impact Caspase-6 Function and Stability"
- Krishnendu Saha (Rotello Group), "The Interplay of Monolayer Hydrophobicity and Protein Corona on the Hemolytic Properties of Nanoparticle"

A whole day with Chemistry and scientific discussions was brought to an end with a delicious cookout served in the beautiful area behind the ISB by the Student Development Committee and graduate student helpers. The BBQ brought the students, faculty, staff, and their families together to socialize.



Ambata Poe, Jeffrey Lucas, Stephen McCarron, Scott Eron, Ryan Landis, Cornelius Taabazuing, Bay Serrano, Kevin Dagbay, and Krishnendu Saha

We gratefully acknowledge the financial support we received for this event from UMass Amherst Department of Chemistry, Richard & Meryl Brown Scholarship Fund, Marvin D. Rausch Scholarship Fund, Dr. Paul Hatheway Terry Scholarship, William E. McEwen Endowment Fund, Fisher Scientific, 3M and Boehringer Ingelheim, the Graduate Chemistry Association, and alumni support. If you are interested in contributing to this event, please contact Vicki Hubby at vicki@chem.umass.edu

something new and exciting going on. I also always liked being in the lab.

GG: Does the love of chemistry run in your family?

MF: My parents were both educated in Hungary as 'food engineers' which translated into my father being a flavor chemist (he makes flavors), and my mother an analytical chemist in the fragrance field.

GG: Did you have a chemistry set when you were little? **MF:** Nope – I think that by the time I grew up they were deemed unsafe.

GG: What was your worst job ever?

MF: I don't think I ever had (a bad) one... or blocked it out.

GG: What convinced you to go to the grad school you attended?

MF: There's only one Caltech; brilliant people, great resources, and it's really small... On the treadmill at the gym, there'd be Nobel prize winners to your left and your right... then you'd find another in the weight room – that



doesn't happen anywhere else because they wouldn't be caught dead working out in the same space. Not at Caltech. It's a great community.

GG: What did you study for your PhD?

MF: I generated, synthesized, and studied molecules that were able to bind to DNA in a sequence-specific manner and used them to change the expression of cancer-related genes.

GG: What was your proudest moment ever (chemistry related or otherwise)?

MF: When I got my first job offer and I knew I was going to be a professor.

GG: Who do you admire and why?

MF: My parents. They came to the US without having degrees that really translated, without much English knowledge, and they had to escape Hungary without telling anyone, to get here (spending 6 mos in Greece enroute). And I still managed to have a fairly normal childhood.

GG: Who in chemistry and related fields do you admire and why?

MF: Oh man... Alice Ting (MIT, Chemistry)—she does great science (sans the retraction issue, which also speaks to her integrity I think), she gives great talks, she's wicked intense, and she's done it 'her way'.

GG: What is the most useful tool in your lab?

MF: Does the nespresso maker in my office count?

GG: Do you use any novel techniques or tools, or work with any unique materials for your research?

MF: I would say that none of my techniques are new or unique individually, but putting them all together (cell culture, molecular biology, and synthetic chemistry) is.

GG: Do you work in any collaborations?

MF: My lab will be collaborating with several on campus groups in the future, including the Bittman, Jerry, Peyton, and Rotello groups.

GG: Have you ever had a job in industry?

MF: I worked for Bristol-Myers Squibb in medicinal chemistry from 2001-2004, and was part of a team that developed a first-in-class HIV attachment inhibitor.

GG: How does industry impact your science?

MF: I think we're trying a different approach, so it doesn't really at this stage.

GG: Assuming your research is wildly successful, how will it impact society?

MF: We're going to understand, image, and cure cancer.

GG: What are the biggest barriers towards your research being wildly successful?

MF: Funding.

GG: Have there been any major advances in chemistry or the technologies used in research since you were a grad student?/Do you ever find yourself telling your students, "Well, when I was in school, we didn't even have..."?

MF: I wasn't a grad student THAT long ago.

GETTING TO KNOW...-continued

GG: Bio focuses (biochemistry/biophysics-Chen) seem to be all the rage among the young chemists; is this a trend among chemists, in general? What could this be attributed to?

MF: I think there are two major contributors: 1. it's really hard to get funding that isn't applicable to solving a human problem, whether it's powering the planet (energy) or trying to find a cure for a disease; and 2. I think a lot more people want to have a research program that will make a 'difference in the world' as opposed to 'science for science's sake' – but it's hard to tell how much of that desire comes from within versus because of the point made in 1.

GG: Which is more stressful, grant proposals, research or teaching?

MF: Teaching – it's what I've done the least of... But grants can also be stressful...

GG: What do you do when you're not being a chemist? MF: I'm always a chemist (especially in this job), but also I enjoy snowboarding, golf, traveling, and hanging out with my puppy. And wine and beer. (and a good single malt on occasion):)

electronicEXAMS

REDEFINE TEACHING & LEARNING IN UNDERGRADUATE CHEMISTRY COURSES

(excerpt from UMass Amherst IT NEWS-December 2013)

Over the past three semesters 3500 UMass students enrolled in General and Organic chemistry have taken examinations electronically on laptops located in the general chemistry laboratory. Students access test materials using OWL, the secure electronic learning system developed jointly by the UMass Center for Educational Software Development and Chemistry. Overall, students report an improved testing experience, while instructors recognize the positive impact of "eExams" on teaching and learning.

This exciting initiative is being led by Chemistry Lecturers Beatrice Botch, Thomas Whelan, Lara Al-Hariri, Christopher McDaniel, and Hans Mentzen. Scores are available instantaneously and instructors can address problematic areas immediately, often in the very next class session. This results in more effective instruction, which facilitates students' learning and ultimately, their academic success. Gone are the "bubble sheet" exams common in large-lecture courses. Instead instructors have a range of question types (numerical answers, structure drawing, matching, multiple choice, etc.) available to assess student learning. Students report a more relaxed testing experience, with ample seating and far fewer interruptions.



From left to right: Professors Beatrice Botch, Hans Mentzen, Lara Al-Hariri, and Thomas Whelan.

The Chemistry department has long been on the cutting edge of undergraduate educational innovation, and this initiative continues the strong tradition. In redesigning the exam experience, Chemistry Lecturers have effectively used existing resources (laboratory space and OWL) and have leveraged funding to obtain computers, supplies, and development support for this effort. The lecturer team will lead a joint workshop with the Center for Teaching this spring to introduce the campus at large to this initiative.



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DEAR ALUMNI AND FRIENDS OF THE DEPARTMENT OF CHEMISTRY,

We have big plans for the 2014 reunion on Saturday, June 7, 2014. This year's reunion will honor Professors George Richason, Jr. and Richard Stein (details are on page 2). As noted in previous Gazettes, construction of new facilities on campus continues at a rapid pace. The Kaltashov, Maroney and Vachet groups have moved into the new Life Sciences Laboratories. This exciting new facility, built with funding from the Massachusetts Life Sciences Consortium and the University, fosters collaborative research and translates fundamental discoveries to the clinic (see feature article). Come see the changes to your alma mater!

I'm delighted to report that Michelle Farkas has joined our faculty as an Assistant Professor. Trained as an organic chemist with Peter Dervan at Caltech, she will develop and use molecular tools to understand, image, and treat cancer. She is interviewed starting on page 1. The University trustees have recently voted to appoint Vince Rotello as a Distinguished Professor, adding to the numerous national and international honors that Vince has earned in the recent past (which include being selected as both a Fellow of the American Association for the Advancement of Science and a Fellow of the Royal Academy of Science in Great Britain).

On a more somber note, I am sad to report that Professor Bob Weis passed away this past November, after a long battle with cancer (see page 21). Bob joined our faculty in 1988 and was beloved by undergraduate and graduate students alike. A pioneer in UMass biophysical chemistry, he will be deeply missed.

On the teaching front, our recent introduction of electronic exams (eExams) in the large lecture courses has exceeded all expectations in terms of value to both students and faculty – no more bubble sheets! Read about it on page 25. The iCons program has blossomed wonderfully and is proud to graduate its first four year contingent this Spring (read about iCons on page 18).

Finally, we continue to be deeply grateful to all of you who have contributed so generously to our department over the years. Your gifts are invaluable towards improving our teaching and research facilities and providing scholarships to students. With your support, we will forge ahead, pushing the frontiers of knowledge and training top-notch scientists!

Sincerely,

Craig Martin, Department Head

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