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Dear Alumni and Friends of UMass Chemistry,

I am approaching the end of my second year as Department Head, and I can say without a doubt that I am least two times as proud to be serving our Chemistry Department. The last year has not only reaffirmed how excellent our faculty, staff, and students are, but it has further humbled me to learn how outstanding and generous our alumni are. Our former students have gone on to do some truly amazing things in the world, but I have been astounded by their eagerness to give back



to our Chemistry community. As examples, in the last year, two new student awards have been created by alums – the Tarselli Family Research Award and the Thomas R. "Casey" Stengle Scholarship – adding to the amazing support we receive from former students and faculty in the Department. You can read more about Michael Tarselli in this issue of the Gazette. The Stengle Scholarship was started by Dr. Diane Stengle, who is a Chemistry alum and wife of late Chemistry Professor Thomas "Casey" Stengle, who served on the faculty from 1959 to 1993. The Stengle Scholarship is awarded to a chemistry major who has a financial need and maintains good grades. You can also read more in this issue about the recently started William Lee Science Impact Program, which aims to broaden participation in undergraduate research in our College. It is inspiring to see how people who made our Department excellent in past years are still committed to helping us maintain our excellence as we move forward into the future.

Speaking of the future, several of our faculty are moving into an almost futuristic new science building this summer. After years of announcing the forthcoming Physical Sciences Building, I am pleased to report that it opened for occupancy in August 2018. This new building not only provides state-of-the-art research space for synthetic chemists in our Department, but it is very forward-looking in terms of sustainability. As an example, water used for cooling chemical reactions will be re-circulated via a closed loop, meaning very little water in the building will be wasted. There is also a solvent dispensary shared by all the Chemistry faculty in the building, leading to substantial savings in solvent consumption.

Sadly, the year was not filled with all good news. Two of our faculty colleagues passed away. Prof. Howard Stidham, who researched and taught in our Department for over 60 years (!), passed away in November 2017. Howard had a storied past as described in this issue of the Gazette, and I'll never forget the lessons he taught me about scientific writing when I was a brand new faculty member. Our colleague Prof. Paul Dubin also passed away in May 2018. Paul joined our Department in 2005 after many years as a Professor at Indiana University-Purdue University at Indianapolis. I will miss the many spirited scientific discussions that I had with Paul over the years. Both Howard and Paul will be missed by us all.

To end on a more upbeat note, it was an award-winning year for many of our students and faculty. There are too many to list all of them here, but I will highlight a few. Graduate student Ryan Landis won the \$20K Innovation Challenge for his founding of Phytos Therapeutics, which designs nanotechnological solutions to address infectious diseases; Emil Samson won a prestigious NSF Graduate Research Fellowship, being one of the winners from a pool of over 12,000 applicants; graduate student Christie Ellis won an inaugural CNS Excellence in Diversity and Inclusion Award, recognizing her efforts to promote a climate of diversity and inclusion within the college; and Prof. Jeanne Hardy won the inaugural Mahoney Life Sciences Prize for her research on the protein caspase-6, which is implicated in aspects of Alzheimer's disease. UMass Chemistry certainly has some great people!

Sincerely,

Richard Vachet

depthead@chem.umass.edu

Physical Sciences Building

The 80,000 square foot Physical Sciences Building (PSB) is now open! It provides space for 80 chemistry graduate students and postdocs in 22,000 square feet of state-of-the-art synthetic chemistry labs on Levels 1 and 2, and specialized, "high bay" space for physics on the lower floor. The PSB will be home to 6-8 chemistry research groups, including the Andrew, Kittilstved, Thayumanavan, and Venkataraman groups, who have just moved in (August 2018), as well as new faculty hires.

The building was designed by Wilson Architects and construction was managed by Whiting-Turner. Enhancing collaboration between groups and within a group was a major design goal, as was creating efficient use of space with the flexibility to be readily adapted to meet evolving research needs. The labs feature an open floor plan, so lab space for one group is adjacent to that of another, with no walls between them. In addition to the clear advantages of increasing interactions between groups, this provides the ability for the amount of lab space each group uses to broadly follow changes in group size.

The PSB incorporates numerous green building features and has earned Silver LEED (Leadership in Energy and Environmental Design) certification, which is very challenging for a building with such high air-handling requirements. The extensive windows and glass wall allow natural light to illuminate the labs. Energy-and water-saving features include high-efficiency fume hoods with a hood monitoring system to encourage closing of hood sashes when not in use and a closed-cycle chilled water loop (for stills, etc.). There is open space for specialized instrumentation like glove boxes, and dedicated rooms for high hazard work, solvent dispensing, and mammalian and bacterial cell culture.

The Venkataraman and Kittilstved groups are on the first floor. The Venkataraman group synthesizes novel organic and hybrid organic/inorganic materials for energy harvesting and storage. They are designing new types of metal halide perovskites, with the goal of improving the stability of these promising solar energy collection materials. They also study how the charge is transported in perovskites, which is key to their use as electronic materials. In energy storage, they have recently made a significant advance, achieving the highest energy density to date in a photothermal battery. The device is based on an azobenzene-based poly(methacrylate) polymer which they designed and synthesized. Prof. Venkataraman notes, "The PSB is a boost for collaborative research. It will help foster a dynamic research community in synthetic and materials chemistry. My research group will share the lab corridor with Prof. Kevin Kittilstved's group, which will allow our groups to interact on a daily basis and exchange ideas. These interactions will lead to exciting and transformative science."

The Kittilstved group develops methods to synthesize novel inorganic materials for renewable-energy applications and spin-based technologies. The materials are primarily inorganic semiconductors and related molecular clusters with controlled doping that confers novel magnetic, electronic and optical properties. Please see p. 9 for more on their research. "The main thing that I'm excited about with the move to the PSB is that it will enable



Exterior view from East Experiment Station vantage point



Open lab design and common spaces enhance interdisciplinary research and facilitate collaborations



Student writeup desks, adjacent to the labs, separated by a glass wall, to allow for monitoring of ongoing reactions



Modular labs, with a hood, bench space, and shared sink



Central solvent purification and dispensing stations are convenient and allow purchasing in bulk



View of the Integrated Sciences Building from the PSB conference room



David Bilger (Andrew group) in front of physical vapor deposition chamber



Custom rotovap cabinet



Goessmann and the new West Experiment Station

new interactions between students and faculty as well as strengthen existing collaborations among chemists, and also with physicists. This is a win-win for materials chemistry and I am looking forward to welcoming new faculty in 2019," says Prof. Kittilstved.

The Thayumanavan and Andrew groups share the second floor. The Andrew group designs and synthesizes organic molecules that they polymerize (or in some cases, crystallize) to produce materials with useful electrical, optical and magnetic properties. Applications include wearable electronics, high-resolution optical lithography, and magnetic tunnel junction devices. Their research is described in more detail on page 8.

The Thayumanavan group is the largest group moving into the PSB, with 22 graduate students, a postdoctoral fellow and a Research Assistant Professor. The Thayumanavan group designs and synthesizes small molecules and polymers that self-assemble into nanoscopic systems with the capability of autonomously responding to specific microenvironments. Such capabilities have impact in a variety of applications, ranging from engineered self-healing materials to nanomedicine. In the area of nanomedicine for example, the group is interested in delivering therapeutic small molecules or biologics to specific tissue targets with implications in many diseases, especially liver diseases and oncology. Prof. Thayumanavan and members of his group are thrilled with the new space, "The exciting aspects about the PSB move are multi-fold. The building has an openlab space plan that fosters collaboration among the students within the group; it is more centrally located between our collaborators' labs, which is ideal for enhancing efficiencies in our collaborative research; and the more modernized facilities offer an overall better and safer setting for cutting-edge research. For our own research group, it brings all our team-members into a single lab space, which we are particularly excited about."

With its many state-of-the art, adaptable and user-friendly features, the PSB will inspire students, postdocs and faculty, and will foster interdisciplinary and collaborative research for decades to come.



Rear entrance to the PSB and WES connection



Goessmann and PSB 2nd floor connection



View from the Campus Center



WES, Lederle Tower, and PSB

faculty Highights

Thayumanvan Lab Celebrates Six Successful Women Graduates

The percentage of women in STEM fields is increasing, but especially in the physical sciences, there is still progress to be made. The "Thai" Thayumanayan lab



recently celebrated a success as six female students (Youngju Bae, Mallory "Molly" Gordon, Celia Homyak, Oyuntuya Munkhbat, Priyaa Prasad, and Poornima Rangadurai) received their advanced degrees at Graduate Commencement on May 11. Thai says, "It didn't dawn on me until we were there at the ceremony, but suddenly I realized 'Wow!' We have done something really amazing here."

Rotello and International Colleagues Develop New Blood Test to Detect Liver Damage



Vincent Rotello and colleagues at University College London (UCL), U.K., announced that they have developed a "quick and robust" blood test that can detect liver damage before symptoms appear, offering what they hope is a significant advance in early detection of liver disease.

Liver disease is a leading cause of premature mortality in the United States and

U.K.; it often goes unnoticed until late stages of the disease when the damage is irreversible. The newly developed method can detect liver fibrosis, the first stage of liver scarring that can lead to fatal disease if left unchecked, from a blood sample in 30-45 minutes.

Thayumanavan Lab Develops Molecular Switch for On-demand Release of Molecular Cargo



Sankaran "Thai" Thayumanavan and colleagues at the University of Massachusetts Amherst have shown for the first time how movement of a single chemical bond can compromise a membrane made up of more than 500 chemical bonds. Their system uses light as a switch to create a reversible, on-demand molecular control mechanism. Details

were published in Nature Chemistry.

Thayumanavan, Minter Focus on Drug Delivery System for Rheumatoid Arthritis

S. "Thai" Thayumanavan, along with Professor of Animal Science Lisa Minter, have partnered with Anika Therapeutics Inc. of Bedford to co-develop a new product for treating the autoimmune disease rheumatoid arthritis. They and the company will focus on research to optimize a drug delivery system to advance a new therapy candidate. The work is part of Phase II of a continuing relationship between IALS (Institute of Applied Life Sciences) and Anika.

Jackson and Beck Research Groups Spatially Resolve Catalytic Activity on Metal Surfaces

The Jackson Research group, along with an international team of researchers, have used infrared spectroscopy techniques and a quantum theory model for a more complete understanding of methane dissociation reactions on platinum. The results were featured in *The Journal of Chemical Physics*.



Thompson Awarded NIH Grant to Study Chemotaxis Receptor Signaling Complexes

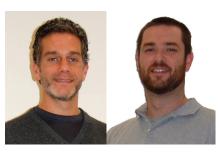


Lynmarie Thompson was awarded a two year, \$615,000 NIH grant entitled, "Assembly and Function of Bacterial Chemotaxis Receptor Signaling Complexes." The goal of the project is to assemble native-like functional nanoarrays of chemotaxis receptor complexes and determine how the proteins change their structure and

dynamics during signaling. Understanding signaling in this system may be useful for the development of novel antibiotics targeting similar signaling systems that are widespread in bacteria.

Auerbach and Schnarr Awarded University Distinguished Teaching Award

Scott Auerbach and Nathan Schnarr have each been awarded the UMass Amherst Distinguished Teaching Award (DTA), the campus's highest honor for teaching.

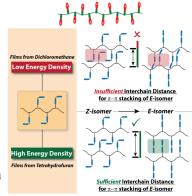


Scott Auerbach

Nate Schnarr

Venkataraman Group: A Polymer Chain Organized Like a String of Christmas Lights Assists Energy Storage

Dhandapani Venkataraman, with PhD student and first author Seung Pyo Jeong, along with PhD students Larry Renna, Connor Boyle, and others, report that they have developed a polymer-based system that can yield energy storage density more than two times higher than previous polymer systems.



Details appear in *Scientific Reports*.

and Virtual Reality to enhance the learning experience for STEM students.

an inclusive syllabus design as a panelist in a workshop

sponsored by TEFD. Al-Hariri and colleagues in the Biochemistry and Physics Departments are collaborating to

develop innovative teaching techniques using 3D printing

Rotello's Nanoparticles Resurrect Antibacterial Drugs

Vincent Rotello's research using nanomaterials as vehicles for drug delivery could be a way to help prevent bacterial resistance to antibiotic drugs. His work explores how surface functionality of nanomaterials could be used to target bacterial infections.



Auerbach Awarded the CNS Outstanding Service/Outreach **Award**

Scott Auerbach was the 2017 recipient of the CNS Outstanding Service/Outreach award, which recognizes and honors faculty excellence and achievement in service and outreach.

Gierasch Winner of the Ralph F. Hirschmann Award in Peptide Chemistry



Lila M. Gierasch received the Ralph F. Hirschmann Award in Peptide Chemistry for her seminal contributions to peptide structure and function, peptide models for protein folding and function, and roles of peptide and protein aggregation in disease.

Maroney Honored at 2017 Faculty Convocation



Michael Maroney was one of eight faculty who received the Award for Outstanding Accomplishments in Research and Creativity at the 13th Annual Faculty Convocation on Wednesday, October 11, 2017 at the Campus Center Auditorium.

Al-Hariri Selected as 2017-18 TIDE Ambassador Lara Al-Hariri was awarded the TIDE (Teaching for Inclusiveness, Diversity, and Equity) Ambassadors Fellowship



as part of the 2017-2018 cohort. The TIDE Ambassadors participate in a yearlong faculty learning community to explore how they can enhance students' learning success across cultural, social, and learning differences. She incorporated inclusive pedagogical practices into many aspects of her courses and shared her experience in using the principles of

Vachet Receives Grant to Study, Prevent Protein Aggregation

Richard Vachet received a four-year, \$1.2 million grant from the National Institutes of Health to continue his group's study of the aggregation by β -2-microglobulin (β 2m), the protein that forms amyloid fibril deposits in the joints of patients with kidney disease who are undergoing dialysis.



Vachet and colleagues will develop new measurement tools using mass spectrometry to understand the molecular details associated with β 2m amyloid formation and will apply this understanding to study potential drugs that could stop this process.

Thayumanavan Receives \$1.8 Million for Center for **Autonomous Chemistry**

Sankaran "Thai" Thayumanavan, has received a three-year, \$1.8 million grant from the National Science Foundation to create a multi-university Center for Autonomous Chemistry, where he and colleagues including Vince Rotello, will seek to design artificial self-activating systems.

graduate student Accomplishments

Elvan Cavac wins the Grinspoon Entrepreneurial Spirit Award for Pickmeup Snacks



Elvan Cavac, from the Martin Group, won the Grinspoon Entrepreneurial Spirit Award for her start-up, Pickmeup Snacks, which uses cricket protein to create healthy and sustainable treats.

Elvan says, "Our vision is that bugs will be a staple in our kitchens, and we will eat

more of them than beef or pork. Pickmeup Snacks are nutrient dense, high protein snacks made with cricket protein powder, and they are also really delicious." Check out her snacks products at https:// www.pickmeupsnacks. com/



Christie Ellis Wins AAAS Mass Media Fellowship



Christie L.C. Ellis, a doctoral candidate in the Venkataraman research group, has received a Mass Media Fellowship from the American Association for the Advancement of Science (AAAS). The fellowship will support an internship this summer at the St. Louis Post-Dis-

patch, where she will work as a science writer.

Ryan Landis \$20K Innovation Challenge Winner

Phytos Therapeutics, headed by Ryan Landis (PhD student in the Rotello group), won \$20,000 in the Innovation Challenge, hosted by the Berthiaume Center for Entrepreneurship. Phytos Therapeutics designs, develops and licenses groundbreaking nanotechnology to address the growing



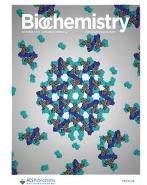
dangers of infectious disease.The seed money will allow Phytos to rent space in IALS co-laboratories facilities where they can continue R&D in collaboration with the Stockbridge School of Agriculture.

Christie Ellis Wins CNS Excellence in Diversity & Inclusion Award

The CNS Excellence in Diversity and Inclusion Awards recognize and honor excellence and achievement in promoting a climate of diversity and inclusion within the college. Christie Ellis demonstrated leadership and innovation in increasing, retaining, and supporting the success of individuals who have been historically underrepresented in CNS and/or in removing the barriers that prevent full participation of all members of our community.

Haglin's Work Featured on the Cover of Biochemistry

Graduate student Elizabeth (Libbie) Haglin from the Thompson group, Chemistry, and Models to Medicine (M2M), IALS, has been featured on the November 2017 cover of Biochemistry for her work on chemotaxis receptors.



In bacteria, chemotaxis receptors (gray) spontaneously assemble with the kinase they control (blue) and a coupling protein (cyan) into a mem-

brane-bound hexagonal array (rendered in this illustration from PDB entry 3JA6). This array enables bacteria to sense molecules in the environment and transmit signals that direct swimming. The full citation: "His-Tag-Mediated Dimerization of Chemoreceptors Leads to Assembly of Functional Nanoarrays." Biochemistry 56 (44), 5847-5966 (2017).

Emil Samson Wins NSF Graduate Research Fellowship



Emil Samson, a first-year graduate student in the Thayumanavan lab, received a National Science Foundation Graduate Research Fellowship (NSF GRFP). His current research project aims to develop molecular design guidelines towards autonomous

systems that can mimic complex systems in nature. Samson is designing an amphiphilic expansile nanogel (eNG) to mimic the binding activities between surface ligands on white blood cells and sugar molecules within the blood capillaries.

Bib Yang Receives Eli Lilly/WCC Travel Award

The Women Chemists Committee (WCC) of the American Chemical Society announced that Bib Yang (Min Chen group) is one of 10 national recipients of the Eli Lilly/WCC Travel Award.



Promotions Promotions

Assistant Professors **Trisha Andrew**, **Min Chen**, **Kevin Kittilstved** and **Eric Striete**r have been recommended for tenure and promotion to Associate Professor by the Provost, and approved by the Board of Trustees. Their promotions will take effect September 1, 2018. Associate Professor **Jeanne Hardy**'s promotion to Full Professor has been approved by the Chancellor and Provost and will also take effect September 1.

Trisha Andrew

Prof. Andrew joined the UMass Amherst Chemistry department as an Assistant Professor in 2016, moving her lab from the University of Wisconsin. She has ongoing research endeavors to 1) create solar textiles and other monolithically-integrated wearable technologies using vapor phase organic



chemistry; 2) effect subdiffraction optical lithography using organic photochromes; and 3) synthesize organic analogs of diluted magnetic semiconductors. Her group is best known for textile-based electronic devices. These are made possible by their development of oxidative chemical vapor deposition methods to uniformly and conformally coat a biocompatible conducting polymer onto the surface of a variety of off-theshelf textiles. Devices they have created include fabric electric heaters (for self-warming gloves) and conductive garments capable of acting as biocompatible electrodes for personal health monitoring. They have also harnessed the triboelectric effect - charge generation induced by two different materials rubbing against each other – in several creative ways. They have created textiles that produce an immediate touch response and can distinguish finger pressure, touch duration and gesture, similar to a capacitive touch screen. Their textile-based triboelectric generators are capable of differentiating different kinds of small body movements (for health monitoring), and they are developing triboelectric generators to charge portable electronics (such as cell phones) using electricity generated by incidental movement of the user's garment.

Jeanne Hardy

Prof. Hardy joined the faculty of the University of Massachusetts as an Assistant Professor in Fall 2005 and was promoted to Associate Professor with tenure in 2012. This year she was promoted to the rank of Professor for her work on protease



chemistry and mechanisms. In particular, Prof. Hardy's work focuses on identifying and exploiting novel allosteric sites in biomedically important proteases, the enzymes that cut and thereby regulate other proteins. Allosteric sites, sites distal from traditional drug binding sites (the catalytic or active sites), can often be exploited for more specific drug binding and function with greater precision and fewer side effects. The Hardy lab (https://hardylab.chem.umass.edu/) uses allosteric sites to regulate protein function, to make novel drugs for treating diseases of societal importance and to understand important biological pathways. To date they have identified structural details and mechanisms that are critical for our understanding of how cells regulate the balance between life and death. This is important in diseases like cancer. They have also developed methods for delivering proteins that can effectively kill cancer cells. Hardy Lab also works on a protease that is important in Alzheimer's Disease and developed the most potent and selective inhibitors of that protein that have ever been reported. They also study the proteases from Dengue, Zika and Chikungunya Viruses with the aim of improving antiviral therapy for these infectious agents.

Min Chen

Prof. Chen started as an Assistant Professor in the Chemistry department in 2010. Her research focuses on the structure, dynamics, and function of pore-forming membrane proteins. She then employs these insights to create diagnostic analytical technologies derived from engineered pore-based nano-sensors. The primary tool her group uses is electrophysiology, in which they measure the current flowing through a single membrane protein embedded in a lipid bilayer with excellent current and temporal resolution. The current flowing through a pore under an applied potential is altered when an analyte binds to the pore-forming protein. The frequency of the binding events allows the determination of the concentration of an analyte, while the nature of the events (their amplitude or duration) enables analyte identification. Compared to other approaches, this stochastic sensing has the advantage of being sensitive (nanomolar concentrations), fast (up to microsecond resolution), and without delays from mixing and diffusion (real-time). Using this approach, she has developed a high-throughput method that quantifies cell penetrating peptide-mediated

and guide the development of the next generation of drug delivery systems.

protein delivery. The technologies created in her lab have the potential to both greatly accelerate sensor design and deployment

Kevin Kittilstved

Prof. Kittilstved joined the UMass Chemistry department as an Assistant Professor in January 2011. His research is focused on understanding and manipulating the electronic structures of transition metal ions in inorganic hosts for a wide range of



applications such as solar energy conversion, photochemical water splitting, and spin-based electronics. This is accomplished by synthesizing inorganic materials across a wide range of length scales from the nanoscale to the bulk. To correlate the function of these multifunctional inorganic materials with the electronic structures of the transition metal ion his group employs sophisticated characterization techniques including high-resolution electronic absorption, luminescence, and magneto-optical spectroscopies. A signature accomplishment is his ability to introduce transition metal ions into specific sites in semiconductor nanoclusters. The interactions between these targeted dopants and band carriers in the semiconductors enable new functionality within inorganic materials, such as reversible electron storage leading to supercapacitance.

Eric Strieter

Prof. Strieter joined the UMass Amherst Chemistry department as an Assistant Professor in 2016, moving his lab from the University of Wisconsin. His research focuses on post-translational modifications in proteins, particularly processes



that target proteins for degradation. Although the human genome encodes for 20,000 proteins, the human proteome consists of at least 200,000 and up to 2 million distinct protein forms. This additional complexity is due to post-translational modifications (PTMs), covalent modifications to the side chains of amino acid residues in proteins. PTMs consist of the covalent attachment of both small molecules (phosphate, methyl, glycosyl, or acetyl) and proteins, e.g., ubiquitin and ubiquitin-like molecules. The PTM networks are intertwined, and miscues can lead to the development of immune disorders and cancer. The Strieter group uses synthetic organic, analytical and biochemical tools to understand the molecular details of how specific enzymes activate ubiquitin and related proteins, attach them to specific amino acids in the target proteins, and even attach additional ubiquitins to existing tethered ubiquitins to form linear and branched chains. Complementary enzymes remove ubiquitin, forming a complex biochemical network. Understanding these processes is not only critical for the development of new therapeutics but also for the functional interpretation of mutant forms of enzymes that lead to human disease.

Faculty

Amanda Bennett

Amanda Bennett, who supports the general and organic chemistry teaching labs, will be teaching Writing in Chemistry as a Lecturer for the department. Her eclectic background – she has Bachelor's degrees in both Chemistry and English from Hamilton College and an MFA in Creative Writing from Boise State University – will be particularly useful in this role, as will her ten plus years teaching composition and writing courses.

Tais Labrador

Tais Labrador will be starting as a Visiting Assistant Professor in Fall 2018. She earned her PhD in physical chemistry from the University of Colorado, Boulder in 2018, using steady state and time-resolved spectroscopy to measure how ligands affect the photophysics of nanocrystals. She will be teaching in the General Chemistry sequence.

Xueying (Sharon) Qin

Xueying (Sharon) Qin joined the department as a Lecturer in Spring 2017. She earned her PhD in 2007 from the Univer-

sity of California, San Diego, studying aerosols and their effects on climate and health. She continued to pursue these interests as an Environmental Scientist at the Kansas Department of Health and Environment. She came to UMass from Kansas State University, where she was



an Instructor in the Biochemistry and Molecular Biophysics department. She has taught both semesters of non-majors General Chemistry, as well as the one-semester versions of General and Organic Chemistry.

Rachid Skouta

Rachid Skouta will be joining the department as a half-time Lecturer in Fall 2018. He earned his PhD in 2008 from McGill University, then was a post-doctoral fellow and later a Research Associate at Columbia University. He comes to UMass from the University of Texas El Paso, where he was a non-tenure track independent Principal Investigator doing medicinal chemistry, primarily discovering small molecule drug candidates to combat lung cancer. He will be teaching non-majors Organic Chemistry.

Sravan Surampudi

Sravan Surampudi will be starting as a Lecturer in Fall 2018. He earned his PhD from UMass Amherst in 2013 (working with Prof. Venkataraman), synthesizing conjugated molecules with novel optical and sensing properties, then was a teaching postdoctoral fellow at Johns Hopkins University. Since



Spring 2016 he has been a temporary lecturer in the UMass Chemistry department. He will continue to teach non-majors General and Organic Chemistry.

Notes Notes

Auerbach Group

The Auerbach group had a banner year in 2017 in research, teaching, and service. The Auerbach group made significant research breakthroughs in modeling the self-assembly of nanoporous materials such as zeolites and mesoporous silica materials. Zeolites are the most used catalysts by weight on earth and offer the potential for 21st-century applications in carbon dioxide capture and renewable biofuel production. The present and future applications of zeolites arise from their nanoporous crystalline structures. Despite the great importance of zeolites, zeolite chemists still rely heavily on trial-and-error in their search for new materials, because the mechanisms controlling zeolite formation remain poorly known. Understanding such mechanisms will be critical to one of the "holy grails" of materials science - rational design of tailor-made nanoporous materials. In two papers published in 2017, the Auerbach group (with longtime UMass collaborator **Prof. Peter Monson**) developed and applied new computational chemistry techniques to solve two key problems: (i) understanding how pores are formed during zeolite crystallization, and (ii) determining the role of silicate bonding during mesopore formation. The first paper features **Dr. Cecilia Bores** as first author; Dr. Bores is now doing a postdoc at the University of Texas, learning how to model protein structures. The second paper features **Dr. Szu-Chia Chien** as first author; Dr. Chien is now a research professor at Ohio State University. This research is funded by the Department of Energy because nanoporous materials have the potential both to generate sustainable fuels, and to save energy in the chemical industry with energy-efficient separations.

Prof. Auerbach's educational work on the UMass iCons Program – a signature science program for UMass Amherst undergraduates that challenges interdisciplinary teams of students to tackle real-world problems in biomedicine and renewable energy - was on vivid display in 2017. Prof. Auerbach gave invited keynote addresses and held faculty development workshops at Worcester State University, Middlebury College (Vermont), UMass Medical School in Worcester, the Howard Hughes Medical Institute Professors Symposium (Maryland), and at the New England Association of Schools and Colleges Annual Meeting in Boston. Prof. Auerbach won several awards in 2017 for his educational innovations in Chemistry and iCons, including the UMass Amherst Distinguished Teaching Award (the highest teaching award given at UMass Amherst), the Chemistry Department Distinguished Teaching Award (determined by Chemistry undergraduates), and the UMass College of Natural Sciences Outstanding Service Award (for leading the creation of the

iCons Program). To read more exciting news about the UMass iCons Program, please see page 22.

This has also been a terrific year for alumni of the Auerbach group. **Dr. Hongbo Shi** graduated in 2017 with a PhD in Chemical Engineering, and has taken up a research position at the world-class semiconductor company GlobalFoundries in Santa Clara, CA. Dr. Angela Migues (PhD, 2016) has accepted a faculty position in the Chemistry Department at SUNY Oneonta, to begin in September 2018. Dr. S. Vaitheeswaran (postdoc) has taken a teaching positon in Physics at Framingham State where he will apply his unparalleled enthusiasm to introduce young minds to the wonders of classical and modern physics. And finally, Dr. Hari Ramanan (PhD, 2006) has taken a teaching position at the Rishi Valley School in Andhra Pradesh, India, which shares with the UMass iCons Program many aspects of its educational philosophy. We wish all of these Auerbach group alums good fortune and success as they enter into the next chapters of their lives and professional careers.

And we wish all Auerbach group alums a wonderful year, and hope they'll stay in touch and visit campus whenever possible. Remember: Go CRUNCH = Chemistry Research Using Nice Computer Hardware!

Barnes Group

This year, **Prof. Mike Barnes** continued research with a new collaborative grant from the National Science Foundation with support totaling \$450,000 (through 2021).

Prof. Barnes gave an invited presentation at the University of Rochester. The Barnes group also had several papers published, including a paper in the prestigious ACS Journal *Nano Letters* on using electric-force scanning probe techniques combined with photoluminescence imaging to reveal "dark" (ground-state) interactions in crystalline organic semiconductor nanoclusters.

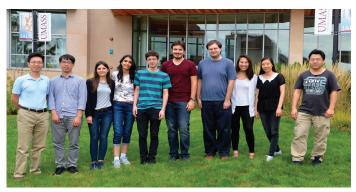
Our group members and research news:

Sarah Marques (5th year Chemistry) won a STEM-Diversity graduate fellowship for AY2019, and Peijian Wang (5th year Physics) received the PhD in Physics at Graduate Commencement in May 2018. Joelle Labastide, (PhD 2015 "Photophysics of Semiconductor Aggregates") was awarded a AAAS Policy Fellowship in Washington, D.C. for 2019. Nick Hight-Huf is a new graduate student in the group, starting in January 2018. Kevin Early (PhD 2010 "Photophysics of Hybrid Quantum Dot-Conjugated Organic Nanostructures") is at 3M Corporation in Minneapolis MN where he heads the Quantum Dot Display laboratory. Michael Odoi (PhD 2010 "Time-resolved Single-Molecule Spectroscopy of Semiconductor Quantum Dot-Conjugated Organic Hybrid Nanostructures") leads a product

development team at Perkin-Elmer Corp. in Bridgeport, CT. **Austin Cyphersmith** (PhD 2012 "Probing Effects of Orientation on the Chiroptical Properties of Single Molecules") is now a Microscopy and Imaging Laboratory Manager at the University of Illinois-Urbana Champaign. **Ruthanne Hassey Paradise** (PhD 2009, "Chiroptical Spectroscopy of Single Molecules"), is a Senior Lecturer at UMass Amherst, and supervises the Analytical and Physical Chemistry Laboratories for undergraduates.

J. Chen Group

2017 has been a busy and exciting year for the Jianhan Chen lab with many important changes. The most exciting of all is the relocation to UMass Amherst in January 2017 from Kansas State University! We have had a lot of help from the wonderful staff in Chemistry, Institute for Applied Life Sciences (IALS), and UMass central IT, and the lab was able to get to full speed and running within a few weeks! In particular, we were able to acquire and set up a new 44node GPU cluster (*Pikes*, housed in MGHPCC in Holyoke) in reasonable amount of time despite several technical challenges. The Pikes cluster has proven instrumental in enabling us to run atomistic simulations of larger and more complex biological systems and for longer timescales that would not be feasible on traditional CPU-based clusters. Two postdoctoral fellows, Zhiguang Jia and Kuohao Lee, and one graduate student, Xiaorong (Sharon) Liu, relocated to UMass Amherst together with Jianhan. In addition, several new members joined the lab after the move, including a visiting researcher (Azar Farjamnia), two postdoctoral fellows, Dr. Mara Chiricotto and Dr. Charles English (joint with the Gierasch lab), a new graduate student, Mahdieh Yazdani, and two undergraduate students, Katrina Nguyen and Justin Campbell. Both Katrina and Justin graduated in summer 2018 with BS degrees in Chemistry. Jianhan has also helped establish a new Computational and Modeling Core for IALS in 2017, which is currently staffed by a full-time research scientist, Dr. Wayne Liang.



Thanks to the smooth relocation, our research activities have experienced minimal interruption in this past year. We have continued to make exciting progress on several active

projects in the general areas of computational biophysics and biomaterials. The group together has published about ten original research articles on diverse topics, including computational method developments, self-assembling peptides, scattering modeling software, fibril aggregation, simulation of disordered proteins, vaccine design, protein folding, and ion channel gating. The full list of publications can be found on the lab webpage at: http://people.chem. umass.edu/jchenlab. Group members have also presented their work at multiple national conferences including GRC - Proteins (June, 2017), Protein Society Meeting (July 2017), Biophysical Society meeting (Feb 2018) and American Chemical Society Meetings (August 2017 and 2018). Jianhan was also invited to present several departmental seminars including a Brown & Williamson Distinguished Guest Lecture at the University of Louisville. Together with Richard Kriwacki from St Jude's Children's Research Hospital, Jianhan has also co-edited a Special Issue in the Journal of Molecular Biology, titled "Intrinsically Disordered Proteins: Structure, Function and Therapeutics."

One of the most rewarding aspects of relocating to UMass has been new opportunities to collaborate with researchers on campus on many scientific problems of fundamental biological and biomedical significance. In 2017, the Chen lab has been able to start working with several labs in Chemistry and other departments, including Min Chen (nano pore protein capture and sensing), Lila Gierasch (DnaK selective promiscuity), Dan Hebert (disordered domains of EDEM1), Lynmarie Thompson (bacterial chemoreceptor), Ned **Debold** and **D. Venkataraman** (myosin protein modulators), and Jeanne Hardy and S. Thayumanavan (novel chemical switches for controlling protein dynamics and function). We have also established a highly productive collaboration with Jianmin Cui's lab at Washington University in St. Louis on studies of BK channels, and another one with Hunaghe Yang at Duke University on TMEM16-family membrane protein channels and lipid scramblases. Some of these collaborations have already led to new research funding for the lab, including a \$200K grant from the American Heart Association (Debold, Venkataraman and Chen, 2018-21), a \$2.9M R01 grant from NIH (Cui, Chen and Zou, 2018-22), and a \$600K MCB grant from NSF (Chen, 2018-22). Together with two existing NIH R01 grants transferred to UMass from Kansas State University, our fortune in research funding will enable us to continue to aggressively pursue these exciting scientific endeavors.

Gierasch Group

As usual, we in the Gierasch lab had a lively time on many fronts in the last year. Five undergraduate students carried out research in the lab, creating a bustling, enthusiastic mix with graduate student **Joe Tilitsky**, postdocs **Wenli** Meng, Sasha Pozhidaeva, and Charles English, as well as Research Assistant Professor Eugenia Clerico. We bid goodbye to three lab members: undergrads Chloe McCollum and Natalie McArthur (both Biochemistry majors) both completed honors theses and graduated. They are now off to graduate school: Chloe at UC Berkeley and Natalie at Columbia University. Chemistry graduate student Joe Tilitsky completed his research on Hsp70 chaperone/ substrate interactions, obtained his MS degree, and started a new position as Research Associate at Kanyos Bio in Cambridge in September. We wish Joe, Natalie, and Chloe the best of luck.



The Gierasch group enjoying the balcony view from the Life Sciences Laboratories.

The Gierasch lab authored four publications covering many different aspects of our research. These papers resulted from collaborations with many scientists at UMass and around the world: We published an article in *Nature Chemical Biology* in the field of protein folding *in vivo*, based on a collaboration with the Garman lab and with Evan Powers from Scripps; through a collaboration with Jack Freed and colleagues in the field of EPR at Cornell University and Carol Robinson and her colleagues in native mass spectrometry at Oxford University, we reported the nature of the allosterically active state of the *E. coli* Hsp70 chaperone, DnaK, in an article in the *Journal of Biological Chemistry*; also in the study of molecular chaperones, our lab published another *Journal of Biological Chemistry* paper on the allosteric mechanism of



The speakers at the Hirschmann symposium in honor of Lila enjoying a toast at the black-tie dinner. (Names, left to right: Joel Schneider, Karyn O'Neil, Lila's husband John Pylant, Lila, Sheena Radford, Jean Baum, and Alan Berry)

DnaK explored through the use of computational simulations; and lastly, a collaborative paper was published in *Methods in Molecular Biology* describing methods to express and purify alpha-1-antitrypsin from *E. coli*. This last paper was the result of a collaboration with former postdoc **Beena Krishna**, now a faculty member in India, and **Anne Gershenson** and **Dan Hebert**, faculty members in Biochemistry & Molecular Biology at UMass.

As usual, group members presented their research at local meetings (such as the CBI/BMB/BMP Joint retreat held at UMass Medical School), and also Lila traveled around the world presenting the lab's work, for example at the Proteins Gordon Research Conference in New Hampshire, the University of Liège in Belgium, and many more.

A highlight for Lila was her selection to receive the 2018 American Chemical Society Ralph Hirschmann Award in Peptide Chemistry. A symposium was held in April of this year in New Orleans, where the Awards presentation was carried out at a black-tie dinner. It is very exciting that this same award was presented to **Lou Carpino** of the UMass Chemistry Department several years back.

Lila was also kept very busy with her duties as Editor-in-Chief of the *Journal of Biological Chemistry*. She authored seven editorials and launched many new initiatives as part of a broad-based campaign to re-invigorate this venerable journal.

We enjoyed visits from former lab members: **Kate Harris**, former UMass undergraduate student in our lab (CHC '03) now Assistant Professor of Chemistry at Stonehill College, came to visit last summer with three of her biochemistry students to review her notes about manual peptide synthesis, which she was teaching in class. She was delighted to refer back to what she wrote in her lab notebook as part of her thesis here 14 years later! **Weiwei Kuo** (former lab postdoc) visited us last summer and told us about her experience as Research Chemist at US FDA in Detroit, MI. **Karan Hingorani**, MCB PhD, 2016, returned to give the Byron Lecture at the MCB Retreat. He talked about his experiences as a medical student at Boston University Medical School.

Hardy Group

This has been another terrific year for the Hardy Lab. In May **Prof. Jeanne Hardy** was awarded the Mahoney Prize in Life Science for a paper published in PNAS with Hardy Lab alumnus Kevin Dagbay. She presented the award lecture June 19th at the UMass Club in Boston and is featured in the UMass Magazine summer edition. **Bay Serrano** successfully defended her dissertation and published great papers in *Nature Cell Death and Differentiation, Biochemical Journal* and *JBC*. Bay is currently a Post-doctoral fellow with Prof. Charles Weitz at Harvard Medical School. **Carolyn Huang**,

an outstanding undergraduate researcher, was awarded the Henry Little prize for earning the highest GPA (4.0) of the 200 students to graduate from the Biochemistry & Molecular Biology department. She will join the Molecular & Cellular Biology graduate program at UC Berkeley in the fall. Post-doctoral fellow Narasimharao Meka designed and synthesized the most selective and most potent caspase-6 inhibitor that has been reported to date. Further testing of its properties for the treatment for neurodegenerative diseases such as Huntington's and Alzheimer's Disease is on-going. Meka completed his Manning Fellowship in the Hardy Lab and is now a fellow in the lab of Brian Blagg at Notre Dame University.



This year we welcomed a new graduate student, Kristalle Cruz, from the University of the Philippines, who is off to a fabulous start, developing a new project on emerging viral proteases. Ishan Soni, a current CBI fellow, received the Protein Science Young Investigator Travel Award for the 31st Symposium of the Protein Society in Montreal, Canada to present his work in collaboration with ActivX BioScience *Inc.* on the functional implications of caspase-6 regulation by various nucleotides. As an NIH BTP fellow, Francesca **Anson** completed a successful industrial internship at Medimmune and coauthored several papers with members of the Thayumanavan lab. Maureen Hill won the Dr. Paul Hathaway Terry Graduate Scholarship Award for an Outstanding ResearchFest Presentation on the specificity and function of Zika virus protease. Derek MacPherson coauthored an excellent paper with Alumnus Scott Eron elucidating the inhibitory interactions of zinc with caspases involved in cell death. Both Maureen and Derek plan to defend their dissertations this summer.

This year Hardy was appointed director of the NIH-funded Biotechnology Training Program (http://btp.umass.edu) and became a member of the NIH MSF-A study section. Alumnus **Kevin Dagbay** was hired as a scientist at ScholarRock, joining fellow Hardy Lab alumnae **Samantha Nicholls**. Alumnus **Elih Velazquez** was promoted to the rank of Lieutenant at in the Biological Defense Research Directorate of the Naval Medical Research Center at Frederick MD.

Jackson Group

Our group continues to explore the dynamics of gas-surface reactions, with a focus in recent years on understanding methane dissociation on transition metal-based catalysts. This is the rate-limiting step in the steam reforming of natural gas. We have developed quantum mechanical methods that allow us to compute the dissociative sticking probability of methane as a function of the translational energy and vibrational state of the methane and the temperature of the metal. Graduate student **Han Guo** has been examining CH. reactions on stepped Ni(211) and Pt(211) surfaces, with an initial recent publication in J. Phys. Chem. Letters. It has long been suspected that the reactivity on "real" catalysts is dominated by reactions at step edges and other defect sites, and we proved this, in collaboration with an experimental group at EPFL (Lausanne, Switzerland). Recently published in *J. Chem. Phys.*, this work was selected by the editors to be promoted on their journal homepage and on the cover as a "Featured Article," and the American Institute of Physics issued a press release. Graduate student **Azar Farjamnia** has been examining the vibrationally inelastic scattering of CH₄ from Ni(111) in collaboration with the experimental group at EPFL. She successfully defended her PhD thesis in the fall of 2017, and Han will defend hers this summer. Working with his collaborators in Toulouse, Prof. Jackson organized and received funding for a CECAM Workshop, "Challenges in Reaction Dynamics of Gas-Surface Interactions and Methodological Advances in Dissipative and Non-adiabatic Processes," held last summer in Albi, France.

Kaltashov Group

2017 was a very busy year in the Kaltashov laboratory, which included publication of five papers, as well as several presentations given by the group members at numerous scientific meetings and conferences. The group received funding from the National Science Foundation to develop experimental strategies based on chromatography and mass spectrometry to study transient processes involving biological macromolecules. Yunlong Zhao defended his PhD dissertation and moved to Regeneron Pharmaceuticals (Tarrytown, NY). A new graduate student, Yang Yang, joined the group in December 2017. The group also hosted two visiting scientists, Jun Liu and Guang-xian Liu (from the State Key Laboratory of Food Science and Technology at Nanchang University in China). A Postdoctoral fellow from St. Petersburg State University, Russia, Dr. Vanda **Liadinskaya** started working with the group in December.

Kittilstved Group

2017 and the first half of 2018 have provided many interesting research discoveries and changes to the Kittilstved group. Kevin was awarded 3 new NSF grants in 2017. The first award

was a renewal of the *Collaborative Undergraduate Research in Energy (CURE) REU* program that was started back in 2007 by **S. Thayumanavan** and recently led by **Justin Fermann**. Taking over as co-PI for the renewal is Senior Lecturer **Ruthanne Paradise**. Kevin attended a PI meeting on the Chemistry REU program in San Antonio in July 2018. The second award was also a multi-investigator award through the Major Research Instrumentation program and will bring a new state-of-the-art powder X-ray diffractometer with the ability to measure samples under non-ambient conditions to campus. This new instrument will enable researchers in chemistry and across campus to monitor the structural properties of various crystalline materials as a function of temperature, atmosphere, humidity, and under reactive gases such as methane or carbon monoxide. Finally, Kevin



Muhammad Abdullah, Jillian Denhardt, Fumi Kato, Haneen Mansoor, William Harrigan, Enes Buz, Ekeoma Ibe, Anand Ode, and

was awarded an *EAGER* award that will allow for 2 years of funding his project *Exploration of a New Class of Semiconductor Nanocrystals with Aliovalent Magnetic Dopants.* To say that it was a great year is an understatement. We look forward to building on

the momentum as we move into new space in the Physical Sciences Building.

The group graduated its 3rd PhD in the Summer of 2017 in **Dr. Dongming Zhou**. He accepted an offer and began as a two-year postdoctoral scholar position at his alma mater in China, Zhejiang University. Dongming made many great contributions to the group including 3 first-author manuscripts and an additional 5 co-authored papers with collaborators in chemistry and PSE. We look forward to hearing more about the great work he is doing at Zhejiang!

Remaining members, William Harrigan, Fumi Kato, Jillian Denhardt, Haneen Mansoor, and Muhammad Abdullah "AB", have been very productive in the lab. In 2018, they were joined by Enes Buz who studied at the Koç University in Turkey. They have been very patient waiting for the move to the new building! In addition to ending the year with 6 graduate students, we also said goodbye to two amazing undergraduates: Christopher Roy and Nicholas Russo. Chris graduated with Honors and is headed to the University of Wisconsin for grad school in chemistry. Nick is also headed to grad school, but was a double major in chemistry and physics... he chose condensed matter physics for grad school and will be attending Boston University. We wish Chris and Nick the best!

Knapp Group

The NIH grant focusing on HIF hydroxylase mechanism and engineering was led by the work of Vanessa Chaplin (PhD defense in June). Both Alex Barbato (BS Chemistry, class of 2017) and Michael McKeon (BS ChemEng, class of 2017) completed their Honors theses in the pursuit of modifying hydroxylase function to label proteins; Mike has joined the Navy and Alex is at Cal Tech for her PhD. Two new additions to the lab have notable news: **Isabella Jaen Maisonet** (Class of 2020) received an inaugural Tarselli Family Award for undergraduate research (article about Mike Tarselli and the establishment of his award is on page 33), and Nayana Thimmiah (BS BMB, class of 2018) completed her Honors Thesis on the topic of enzyme inactivation. We were sorry to see Manju Sharma leave, but happy that she has taken on larger responsibilities in the teaching labs. Mike Mingroni was recognized with the graduate TA award in Chemistry, and we welcomed a new member, Ran Duan, into the fold.

Maroney Group

Work in the Maroney lab in the area of bioinorganic chemistry continues with emphasis on proteins involved in nickel homeostasis and the metalloenzyme NiSOD, a nickel-dependent superoxide dismutase. The work on the biochemistry of nickel began with funding from the NIH in 1986, which has supported the work for over 30 years.

Congratulations are in order for **Dr. Heidi Q. Hu** who successfully defended her thesis entitled "The Role of the Metallochaperone HypA in the Acid Survival and Activities of Nickel Enzymes in *Helicobacter pylori*." Heidi, a student in the Molecular and Cellular Biology (MCB) program who hung out with chemists, has joined the staff at Wolfe Laboratories in Woburn, MA. Prof. Maroney relished the opportunity to introduce the latest regeneration of Dr. Hu at her defense.

Next up is **Hsin-Ting** (**Tiffany**) **Huang**, who has completed her data defense and will defend her PhD dissertation in chemistry in the next several weeks. Tiffany was the first student in the Maroney lab to extensively use mass spectrometric techniques to study nickel metalloproteins, and published on the interactions of RcnR, a nickel- and cobalt-responsive transcriptional regulator in the *Journal of Biological Chemistry* (2018, p 324-332).

Priyanka Basak continues to progress in the chemistry graduate program. She attended the Metallocofactors Gordon Research Conference and presented a poster on her work involving the conformational flexibility of HypA and the implications for urease and hydrogenase maturation in *Helicobacter pylori*.

Prof. Maroney took a half-sabbatical in Fall 2017 and spent some of that time in his collaborator's lab in Bologna, Italy. He was invited to give a talk at the Italian Chemical Society National Meeting in Paestum, Italy, and was able to travel to visit wineries in Bolgheri and along the Amalfi coast during his stay. His research efforts were recognized by the University Award for Outstanding Accomplishments in Research and Creativity at the faculty convocation in October.

Martin Group

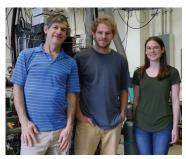
Congratulations to Yasaman Gholamalipour, who presented a poster on her recent work at the Annual Meeting of the RNA Society, in Berkeley, CA. She is working on understanding "problems" in transcription (what we call alternative reaction pathways), so she had a big audience. New understandings from her innovative RNA-Seq studies are leading Elvan Cavac and Kithmie MalagodaPathiranage to develop "fixes" (or what we call alternate reaction and/or process conditions). So we expect an even bigger crowd at future presentations! And of course we're learning a ton about mechanism with this new tool. All three will attend the RNA Therapeutics Conference in late June. Yasaman was also selected as a student speaker at this year's CBI Retreat, and did a great job in her very clear and well-received presentation.

Undergraduates **Kira Chandran** and **Kyle Koczera** are in the area for the summer and are continuing their research projects, while **Adrian Radel** will return next Fall. **Cooper Wharton**, who helped to implement some of the software for analysis of >100,000 sequence data sets, graduated and is moving on to bigger things.

We're very excited to be taking a game changing tool from molecular biology, Next Generation Sequencing, and using it in the analysis of "test tube" reactions. While gel electrophoresis has been a powerful assay for over 50 years, RNA-Seq provides the same (actually, better) information, plus so much more! We anticipate a huge impact in basic science, as well as in the rapidly expanding fields of RNA nanotechnology and RNA therapeutics.

Metz Group

This has been a year with many comings and goings in the Metz group. Congratulations to graduate students **Chris Copeland**, **Muhammad Affawn Ashraf**, and **Dave Johnston**, who all earned their PhDs this year! Chris and Affawn studied the initial step in C-H bond activation by transition metal cluster ions, using vibrational spectroscopy of metal cluster ion complexes with methane and ethane to determine the extent to which binding to the metal weakens the C-H



Rick, Schuyler Lockwood, and Justine Kozubal

bonds. Chris is working for Cyprotex, while Affawn is working for Intel. Dave greatly improved our photofragment imaging instrument and used it to measure bond strengths and photodissociation dynamics in metalcontaining ions such as MnO+ and Al,+. Second-year

graduate student **Schuyler Lockwood** is further improving the instrument and has extended these studies to NiO⁺. We welcome graduate student **Justine Kozubal**, who along with undergraduate **Tristan Heck** has completed electronic spectroscopy studies of Cr⁺(NH₃) begun by Affawn, and has used vibrational spectroscopy to study competition between metal-ligand bonding and ligand-ligand bonding in Cr⁺(NH₃)_n. Please send a note to let us know how you're doing, or stop by if you're in the area!

Rotello Group

2017-2018 featured comings, goings and many other happenings in the Rotello Lab. Vince finished his fourth year as Editor-in-Chief of *Bioconjugate Chemistry*, with **Federica Scaletti** continuing to run the social media website ("like" us at https://www.facebook.com/bioconjugatechemistry!) Vince has done quite a bit of traveling, with five plenary talks in the US, Japan, France, China, and the Netherlands last year. He was also honored as Guest Professor, National Center for Nanoscience and Technology, Chinese Academy of Sciences.

In early 2017 the group celebrated a milestone, publishing our 500^{th} paper. We are on our way to 1000, with 36 publications in 2017, and Vince's h-index up to 103. The group has continued and new funding from the NIH, along with grants from the NSF and USDA.

Three group members won prizes at the 2017 ResearchFest. Congratulations to Li-Sheng Wang for winning the Marvin D. Rausch Scholarship Award for Outstanding Presentation, and to Joseph Hardie and Yi-Wei Lee for their Outstanding Poster Awards. Ryan Landis was awarded \$20,000 for the company he founded, Phytos Therapeutics, in the finals of the Innovation Challenge, hosted by the Berthiaume Center on April 5th, 2018. In addition, our research work on CRISPR/Cas9-ribonucleoprotein delivery for gene editing and its implication in therapy and cell biology research (by Rubul Mout et at.) has been featured in a highlight-interview video by American Chemical Society (https://www.youtube.com/watch?v=OUnPImiYvKg) and our recent work on degradable polymeric nanocomposite 'sponge' antimicrobials has been highlighted in C&EN (https://cen.acs.org/materials/

nanomaterials/Biodegradable-emulsion-eliminates-biofilms/96/i21).

On the departure side, Rubul Mout, Ngoc Le, Gulen Yeşilbag Tonga and Moumita Ray received their PhDs, with Rubul heading to the University of Washington and Gulen to Harvard Medical School, while Ngoc joined the Cambridge Healthtech Institute, and Moumita recently joined Intel. Visiting scholars Dr. Ruijing Yu, Dr. Wenfeng Shen, Yanwei Ji, Imad Ud Din, Dr. Nipaporn Ngernyuang, Tiphaine Tronchet, Baptiste Duse, Dr. Mine Sulak, Adisak Pa, Dr. Dongyo Zhu and Dr. Juan Qiao have returned home. We have had a strong influx of new faces including Jessa Marie Makabenta, Rui Huang and Taewon Jeon who have officially joined our group as graduate students. Welcome to the group!

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.

Thayumanavan Group

The Thayumanavan Research Group has seen another busy and productive year. Below are a few of the highlights.

We are excited to have new graduate students **Myrat Kurbanov**, **Emil Samson**, and **Peidong Wu** join the group. Emil became a recipient of both the NEAGEP Fellowship Award and the very competitive NSF Graduate Research Fellowship.

Current graduate students, **Francesca Anson** (shared student with Prof. Jeanne Hardy) and **Uma Sridhar**, both participated in internships this past year. Francesca did a spring internship at MedImmune in Gaithersburg, MD. Uma did a summer internship last year at Applied Materials in Santa Clara, CA. Francesca also received a Protein Society Travel Award to present her research at the 32nd Annual Symposium in Boston this past July. The American Chemical Society Division of Polymeric Materials Science and Engineering (PMSE) awarded graduate student, **Kingshuk Dutta** with one of three Best Poster Awards. Graduate student, **Arash Manafirad**, who divides his time between Thayumanavan Group and Dinsmore Group in Physics, was granted a Spring 2018 Dissertation Research Grant from UMass.

We have had quite a number of students graduating since the last update. **Dr. Kishore Raghupathi** graduated last year and is working at Intel in Oregon. In May 2018, we had six women from the group graduate: **Dr. Youngju Bae**, who is currently a Postdoctoral Researcher at UMass Lowell, **Dr. Mallory "Molly" Gordon**, now at Anika Therapeutics in Mass., **Dr. Celia Homyak**, currently at JUST Foods in California, **Dr. Oyuntuya Munkhbat**, now at Berkshire Sterile Manufacturing in Mass., **Dr. Priyaa Prasad** and **Dr.**

Poornima Rangadurai, both at Intel in Oregon. There was a great article by UMass News & Media about the six women successfully graduating from a STEM field at https://www.umass.edu/newsoffice/article/thayumanvan-lab-celebrates-six-successful

In addition to graduating, Dr. Youngju Bae had another reason to celebrate. She and her husband, former Master's student in Thayumanavan Group, **Mr. Dongsik Yang**, had a baby boy, Teo. **Dr. Deepak Vishnu Dharmangadan** welcomed a baby girl, Ahaana, to his family. In other news, current graduate student, **Thameez Koyasseril Yeshiva Mohammed**, just got married. We congratulate him and his new wife, Fathima.



New undergraduates joining the research group this past year were: Antony Abi-Elias, Kevin Bonanno, Jenna Westley and Natalie Williams. The following undergraduate students graduated: Bailey Ingalls, who last spring received a 21st Century Leader Award and is currently at Harvard Medical School; Antony Abi-Elias, Marina Franc and Margareta Ianosi-Irimie all graduated in May 2018. Margareta received the Henry Little Award in Biochemistry and Molecular Biology and is now a student at NYU School of Medicine.

We welcomed **Dr. Partha Addy**, from Boston College, to the group as a Postdoctoral Associate in April. Former post docs from the group include **Dr. Subramani "Subu" Swaminathan**, who left in September to become a Research Scientist at Solvay in India and **Dr. Wei Bai**, who is now a faculty member at Anhui University, China.

Three visiting scholars returned to their home countries after a productive stint in the group: **Dr. Sreenivas Peddolla** to India, **Hatice Secinti** to Turkey, and **Zeno Fickenscher** to Germany. Former visting scholar, **Dr. Cunfeng Song**, is now a post doc at Shanghai Jiao Tong University in China.

The National Science Foundation awarded Professor Thayumanavan funding for a three-year, \$1.8 million Phase I Center for Chemical Innovation. The "CCI Phase I: Center for Autonomous Chemistry" funds a multi-university center including **Professor Vince Rotello**, along with Professor Tim Swager from MIT, Professor Jeffrey Moore from the

University of Illinois, and Professor Anne McNeil from the University of Michigan. **Leyla Keough** also joins us as the Center's Managing Director.

Professor Thayumanavan was also awarded a Distinguished Visiting Professor position at the Indian Institute of Technology at Bombay. He will be spending one to two months in Mumbai IIT sometime over the next two years, as part of this recognition.

The Thayumanavan Research Group expects to move in the near future to a brand new facility, the Physical Sciences Building, next door to Lederle Graduate Research Center. The new building is connected to a completely reconstructed West Experiment Station, as well as to the Goessmann Building and will provide both lab and office space for some of the Chemistry faculty and students, including a large space on level 2 for the Thayumanavan Group. The new building is expected to be LEED Silver certified for green environmental design. We invite you to come visit and take a tour of our new work space.

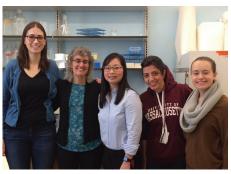
Please visit our website at https://elements.chem.umass.edu/thaigroup/ for more on our news and achievements. Also follow our group on Facebook or Twitter (links provided in our website). If you are a group alum and we do not have your updated whereabouts, please let us know.

Thompson Group

Congratulations to Dr. Libbie Haglin and Dr. Xuni Li! November was a great month for Libbie: she defended her thesis, and her beautiful chemoreceptor assembly was featured on the cover of Biochemistry! Libbie's biochemical experience developing a new method to assemble functional receptor complexes paid off, as she quickly had an interview and job offer at a start-up company. She declined in favor of moving to Seattle with her fiancée, where she will no doubt find a great job. Xuni's experience doing hydrogen exchange mass spectrometry experiments on chemoreceptor arrays (complex samples and complex data!) was key to her obtaining a position as a Research Associate at the UMass Medical School Mass Spectrometry Facility. Shortly after her thesis defense in late January, she bought a new home and moved with her family to start her work there. Lynmarie thoroughly enjoyed having both of them back for graduation!

We welcomed new people to the lab as well. Undergraduate **Kiki Carey** recruited another talented chemistry major, **Tiernan Kennedy** who joined our group in January. They are working together on a new project to use DNA nanostructures for controlled assembly of chemoreceptor arrays. In April we welcomed **Aruni Karunanayake Mudiyanselage** back to the lab. She worked with us previously in 2013 before working with the Martin and You labs. We are happy to have her bring her biochemistry skills

back to our projects as she embarks on hydrogen exchange studies of the kinase controlled by chemoreceptors. In mid-June, **Nikita Mallik** joined the lab, after completing her PhD doing NMR and other biophysical studies of a centromeric



Thompson lab January 2018: Libbie Haglin, Lynmarie, Xuni Li, Maryam Kashefi, Kiki Carey; plus Tiernan Kennedy, not shown.

protein with
Ashutosh Kumar
at IIT Bombay.
Her energy and
experience are a
great addition to
our solid-state
NMR studies of
chemoreceptor
structure and
mechanism.
We also hosted
undergraduate

William Farrell from the University of Dallas for summer research as part of the CURE program, to work on an unusual ABC transporter in a collaborative project with Jeff Blanchard's group.

Congratulations to **Maryam Kashefi** who was selected to speak at the FASEB conference on Molecular Biophysics of Membranes, and also received a Protein Science Travel Award to present her NMR studies of receptor dynamics at the Protein Society Meeting in Boston in July.

Lynmarie co-chaired and spoke in a symposium on transmembrane signaling at the Biophysical Society Meeting in San Francisco in February, and also organized the Molecular Biophysics of Membranes FASEB conference in June. Last summer Lynmarie spoke at both ISMAR in Quebec City and the ACS meeting in Washington DC, and enjoyed reconnecting with **Yael (Amber) Balazs** (PhD 1999) in Washington. Amber has been invited to be the keynote speaker at Researchfest in August 2018!

On the educational front, Lynmarie thoroughly enjoyed a small conference hosted at UMass in January celebrating the 10th Anniversary of Proteopedia, to help brainstorm future directions for using this wonderful tool in education and research. Lynmarie has also been working with Biomolecular NMR Facility Director **Jasna Fejzo** to ramp up the expertise and use of biomolecular NMR at UMass. We started by offering an NMR journal club this spring, to be followed by a Biomolecular NMR course this fall, and have proposed a laboratory module to accompany future offerings of the course.

The Chemistry Biology Interface Program thanks **Nyudlia Araeva** for her work for CBI and we wish her well in her new position as Inclusion and Diversity Coordinator working with Associate Chancellor Anna Branch. We are very happy to welcome **Susan Stinson** as the new Program Coordinator for both CBI and BTP.

Vachet Group

Research in the Vachet group continued in the areas of protein amyloid formation, detection of nanomaterials in cells and tissues, and biomarker detection by mass spectrometry. We also recently expanded our work, developing methods to monitor the structural integrity of protein therapeutics via an SBIR grant with QuarryBio. The group was very productive, having published 12 papers on these topics in 2017 and another 7 so far in 2018. Professor Vachet and his group also made close to 20 presentations at various conferences, meetings, and universities.

In group news, we said good-bye to undergraduate researcher **Nathan Park** who graduated in May 2017 and is now a PhD student at the University of North Carolina-Chapel Hill. More recently, long-time undergraduate researchers **Jennie Paik** and **Tommy Drews** also graduated in May 2018. Jennie will be working in the area, and Tommy is currently hiking the Appalachian Trail.



Current and former Vachet group members at lunch in Indianapolis at the annual American Society for Mass Spectrometry meeting in June 2017.

We welcomed two new graduate students into the group – **Xiao Pan** and **Catherine Tremblay**. Xiao will be further improving our covalently labeling/mass spectrometry approaches for studying protein structure and protein interactions. Catherine will be developing new mass spectrometry methods to study protein therapeutics.

In alumni news, several former students transitioned into new jobs. Myrasol Callaway (MS 2003) took a new position at Regeneron Pharmaceuticals; Feng Wang (PhD 2014) is now a Principal Process Engineer at GLOBALFOUNDRIES; Gokhan Elci (PhD 2017) began as an Assistant Professor in the Biomedical Engineering Department at Pamukkale University in Denizli, Turkey; and Adam Graichen (PhD 2012) is now the Manager of the Mass Spectrometry Facility at UMass. Adam and his wife Allison also welcomed their first child Micah into the world in January 2018. Micah had an [M+H]⁺ of 7 lbs 15.1 oz.

Venkataraman Group

The DV Group had a great 2017-2108 academic year. Seung Pyo Jeong received the top prize at the 2017 ResearchFest, the William E. McEwen Fellowship Award for Outstanding Presentation. **Christie Ellis** received a 2018 AAAS MassMedia Fellowship to work as a summer intern at the St. Louis Dispatch. This fellowship will allow Christie to learn about communicating science to a broader audience. Julia Lenef, an undergraduate in the group, received the 2018 American Chemical Society Organic Chemistry award and the 2018 Connecticut Valley Section of the American Chemical Society Student Award. Julia will be pursuing her graduate studies in Materials Science and Engineering at the University of Michigan Ann Arbor. Matthew 'Donnie' Rollings, also an undergraduate, received the 2018 Mr. Tompkins Award and the Senior Class Award. Donnie will be pursuing his graduate studies in Chemistry at the University of California at Berkeley.

The DV group had a productive year in terms of publications. Our paper on high energy density photo-thermal batteries using azobenzene-based polymers garnered good publicity (DOI:10.1038/s41598-017-17906-w). **Seung Pyo** spent about a year working out several control experiments to probe the origin of the observed high energy density. We also collaborated with Dr. Kwak at Schrödinger Inc to understand the role of molecular packing on energy densities. We also made several advances in the understanding of Perovskite-based solar cells. Using Kelvin probe force microscopy, Larry Renna uncovered the role of active layer-electrode interfaces on the macroscopic polarization in perovskites (https://doi. org/10.1016/j.matlet.2018.01.106). Emily Smith, Christie L.C. Ellis, and Hamza Javaid in collaboration with Prof. Monojit Bag uncovered the interplay between ion transport, applied bias, and degradation under illumination (DOI: 10.1021/acs.jpcc.8b01121). Visit

thedvgroup.com to keep updated on some of the exciting science. Also, the group came up with a new logo and name.

We are now Advanced Laboratory for Iontronic, Electronic, and Nanomaterials. We are now ALIENs! Another significant change will be the location of our lab. We will move into the new Physical Science Building this summer! Memorable events in the LGRT lab: Jay and I painting the hoods by sitting inside the hood, Uche ripping the wall to get

the fire extinguisher, Noah 'painting' the last hood with Pd catalyst, Rattan pleading with physical plant to paint his wall, Tom van der Poll and I arguing about his honors thesis in 1512 ... In PSB, our labs will be next to Prof. Kittilstved's lab. We look forward to new collaborations and science.

From the alumni side, G. (Nag) Nagarjuna is an assistant professor at Georgetown University in Washington DC and for his first independent research grant and publication. Dana Algaier is now an R&D Ink Chemist at Hewlett Packard. She visited us to recruit students from UMass. Larry completed his postdoc with Prof. Shane Ardo at the University of California, Irivine, and is now a scientist at Fisker. Jay Field received the Faculty of Science Distinguished Alumni Award from the University of Waterloo. Jay is the President and CEO of Life Sciences Ontario. Sravan Surampudi is now a lecturer in our department. Tim Gehan is a postdoctoral fellow at NREL in Colorado. Tim and I met during my recent trip to Boulder. DV is proud of your achievements and likes to hear from all of you. So drop a line when you can to dv@ umass.edu. For group updates and news, visit us on the web at thedvgroup.com and follow us on twitter @dvgroupumass or on Instagram at dvgroup_umass.

You Group

This has been a busy but fruitful year for the You Lab. This is our second year here at UMass, and we have started to publish papers and get some grant support. Dr. Bin Zhao, a postdoc in the lab, published our first manuscript in the Journal of the American Chemical Society on intercellular force measurement. This is a quite useful new tool that several mechanical engineering and biochemistry labs on campus have started to collaborate with us on for real mechanobiological studies. A seed grant from the Institute of Applied Life Sciences (IALS) was awarded for this project. Bin and graduate student Yousef Bagheri are now working together on this project, and our 2nd generation force sensors should come soon. Last year, we have also developed another exciting tool to monitor transient lipidlipid interactions on live cell membranes. This is the first time scientists can visualize and quantify these microsecond-range cellular events. This manuscript was published in Nature Nanotechnology.

In addition to these cell membrane tools, our lab has also made progress in the development of sensors for intracellular small molecule and RNA imaging. **Aruni Karunanayake Mudiyanselage**, a research fellow in the lab, demonstrated a highly sensitive way for imaging low abundance RNAs in live cells. The manuscript is currently under revision in *JACS*. In addition, our 2nd year graduate students, **Qikun Yu** and **Rigumula Wu**, will be respectively the first author of two manuscripts describing novel RNA-based sensors for intracellular imaging of antimicrobials and signaling molecules. Based on these RNA sensors, we were recently granted a National Institutes of Health (NIH) R01 proposal to understand the mechanism of antibiotic resistance.

A new graduate student, **Zhining (Jennings) Sun**, joined the lab this year. **Dr. Kewei Ren**, a second postdoc in the lab,

will join us in June 2018. On the departure side, **Jing Shi**, a visiting student, finished her visit and completed her Ph.D. at Tsinghua University. Aruni has left the group and is now a research fellow in the Thompson Lab at UMass. Several undergrads in the lab, **Casey O'Brien**, **Katherine Poisson**, and **Rashad Almadani**, have graduated from UMass. We will miss all of you!



Graduate student **Qikun Yu** was awarded a two-year UMass Chemistry-Biology Interface Traineeship. Undergrads in the lab were also highly successful in receiving awards. Casey was given the Richard W. Fessenden Excellence Award, Departmental Recognition Award, and Bradspies Summer Fellowship. **Mark Leon-Duque** received the Richason Award, Bradspies Summer Fellowship, and Uche Anyanwu Memorial Award. Katherine received the American Institute of Chemists Award and the Distinguished UGTA award.

Finally, Mingxu was selected as the leader of a new Nucleic Acid Delivery theme at IALS. He gave an invited talk at FNANO and presented at the ASBMB National Meeting. In addition, Mingxu will give an invited lecture on DNA/RNA nanotechnology in INSERM, an equivalent of NIH in France, and will organize a two-day Nucleic Acid-based Sensors symposium at the 256th ACS National Meeting in August 2018. Bin presented at 2018 Spring ACS National Meeting on his intercellular force sensors. Most group members have also presented in several local symposiums.

We are looking forward to an even more successful year. Please visit our website at https://elements.chem.umass.edu/youlab/

We want to hear from you!

Reach out to your group so lab news and notes can be up-to-date in future issues!

If you have an accomplishment or a story you'd like to share in our Alumni News section, please contact us at ggazette@chem.umass.edu.

Be sure to keep your address up to date with the Alumni Association Office at www.umassalumni.com.

27th annual ResearchFest

The 27th annual research symposium, ResearchFest, welcomed the incoming first year students last August with the keynote address given by Dr. Rosemary S. Turingan (Martin lab 2006). The event was a huge success thanks to the support of participants, organizers, and sponsors, and featured four oral presentations by graduate students who were selected by a faculty committee through a nomination/evaluation process. Seung Pyo Jeong (Venkataraman group) was chosen to receive the William E. McEwen Graduate Scholarship in Chemistry for his work on "Achieving High Energy Density in Azobenzene-based Materials for Photo-Thermal Batteries: Role of Solvent-Polymer Interactions" Maureen Hill (Hardy group) received the Dr. Paul Hatheway Terry Graduate Scholarship Award for Outstanding Presentation for her work on "The Curious Case of Zika Protease: A Target for Flaviviral Replication." Bib Yang (Min Chen group) received the Marvin D. Rausch Scholarship Award for Outstanding Presentation for her work on "Selective Detection of Protein Homologues by Outer Membrane Protein G." Li-Sheng Wang (Rotello group) received the Marvin D. Rausch Scholarship Award for Outstanding Presentation for "Fabrication of Protein Films for Biomaterial Applications."

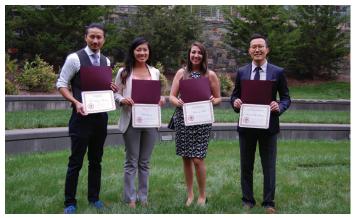
The day concluded with a delicious cookout held in the LSL amphitheater by the Association for Professional Development in Chemistry (APDC – formerly SDC). The BBQ brought students, faculty, staff, and their families together to socialize.

Well over 60 posters were presented this year. The Dr. Paul Hatheway Terry Award for Outstanding Poster Presentation went to Elizabeth Haglin (Thompson Group).

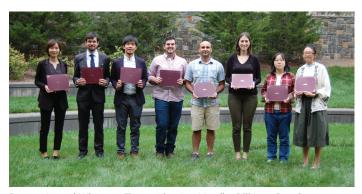
Nine students received William E. McEwen Fellowship Awards for Outstanding Posters: Muhammad Affawn Ashraf (Metz Group), Lin Hui Chang (Streiter Group), Elizabeth Haglin (Thompson Group), Joseph Hardie (Farkas/Rotello Group), Jingjing Gao (Thai Group), Yi-Wei "Bill" Lee (Rotello Group, Hui-Hsien "Tanya" Lin (Farkas Group), Derek MacPherson (Hardy Group), and **Xiao Pam** (Vachet Group).

We gratefully acknowledge the financial support we received for this event from the UMass Amherst Department of Chemistry, Marvin D. Rausch Scholarship Fund, Dr. Paul Hatheway Terry Scholarship, William E. McEwen Endowment Fund, the Graduate Chemistry Association, Graduate Employee Organization, and alumni support. We also thank the following vendors who came to show us what their companies had to offer: ThermoFisher Scientific, Eppendorf, Advanced Cell Diagnosis(ACD), Art Robbins Instruments (ARI), Genesee Scientific, and TCI.

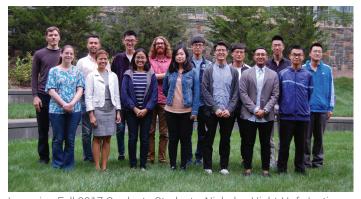
If you are interested in contributing to this event, please contact Vicki Hubby at vicki@chem.umass.edu



Student Speakers (left to right): Li-Sheng Wang, Bib Yang, Maureen Hill, Seung Pyo Jeong



Poster Award Winners: Tanya Lin, Joe Hardie, Bill Lee, Derek MacPherson, Muhammad Affawn Ashraf, Libbie Haglin, Xiao Pan, Lin Hui Chang



Incoming Fall 2017 Graduate Students: Nicholas Hight-Huf, Justine Kozubal, Enes Buz, Jessa Makabenta, Yang Yang, Kristalle Cruz, David Bilger, Yidan Cong, Rui Huang, Kwang Won Park, Peidong Wu, Emil Samson, Zhining Sun, Yanfeng Li, Ran Duan



PhD degrees

Awarded January 2017 - April 2018

Muhammad Affawn Ashraf, "Spectroscopic Studies of Gas-Phase Metal Cation Complexes with Alkanes and Ammonia," Ricardo B. Metz

Youngju Bae, "Light-Harvesting and Light-Responsive Materials for Optoelectronic and Biological Applications," S. Thayumanavan

Christopher W. Copeland, "Spectroscopic Studies of Gas-Phase Transition Metal Complexes of Cations and Cluster Ions with Methane and Water," Ricardo B. Metz

Kevin Buadlart Dagbay, "Probing the Domain Architecture and Structural Dynamics of Caspase-6 for its Specific Regulation," Jeanne A. Hardy

Azar Farjamnia, "Gas-Surface Interactions: Reactive and Non-Reactive Scattering," Bret Jackson

Mallory R. Gordon, "Design and Synthesis of Stimuli-Responsive Polymeric Nanogels Towards Therapeutic Translation," S. Thayumanavan

Elizabeth R. Haglin, "Assembly and Functional Architecture of Bacterial Chemoreceptor Nanoarrays," Lynmarie K. Thompson

Celia Homyak, "Formulation and Characterization of Lipogels as a Tunable Delivery Scaffold," S. Thayumanavan

Jing Huang, "Mechanistic Studies of Peptide-Mediated Protein Transport Across Droplet-Interface Bilayers," Matthew A. Holden

Michael D. Johnston, Jr., "Photofragment Imaging Fast Ion Beams," Ricardo B. Metz

Ngoc Le, "Robust Biosensors for Healthcare Applications: from High-Content Screening to Point-of-Care Testing," Vincent M. Rotello

Xuni Li, "Hydrogen Exchange Identifies Protein Interfaces and Signaling-Related Changes in Functional Chemoreceptor Arrays," Lynmarie Thompson

Rubul Mout, "Protein-Nanoparticle Co-Engineering: Self-Assembly, Intracellular Protein Delivery, and CRISPR/Cas9-Based Gene Editing," Vincent M. Rotello

Oyuntuya Munkhbat, "Role of Rigidity and Flexibility of Functional Groups Within the Interior of Supramolecular Assemblies and Their Implications," S. Thayumanavan

Jake W. Pawlowski, "Novel Mass Spectrometry Methods for the Analysis of Covalent and Non-Covalent Protein Structures and Their Influence on the Functions of Therapeutic Proteins," Igor Kaltashov

Priyaa Prasad, "Design and Development of Redox-Responsive Nanocarriers for Therapeutic Delivery," S. Thayumanavan

Kishore Raghupathi, "Stimuli Responsive Polymeric Nanogels for Hydrophobics and Hydrophilics Delivery," S. Thayumanavan

Poornima Rangadurai, "Study of Self-assembly and Stimuli Responsive Behavior in Polymeric and Dendritic Amphiphiles," S. Thayumanavan

Moumita Ray, "Co-engineering Proteins and Nanoparticles for Fundamental Study and Delivery Applications," Vincent M. Rotello

Banyuhay (Bay) P. Serrano, "The Molecular Basis of Caspase-9 Inactivation by PKA and c-Abl Kinases," Jeanne A. Hardy

Shengsheng Xu, "Analytical Methods to Support Design and Optimization of Protein Drug Conjugate: Focusing on Haptoglobin-hemoglobin Complex as a Drug Carrier," Igor A. Kaltashov

Gulen Yesilbag Tonga, "Nanoparticle as Supramolecular Platform for Delivery and Bioorthogonal Catalysis," Vincent M. Rotello

Yunlong Zhao, "Characterization of Highly Heterogeneous Heparin-Protein Complexes using Novel Mass Spectrometry-Based Approaches," Igor A. Kaltashov

Dongming Zhou, "Aliovalent Dopants in ZnO Nanocrystals: Synthesis to Electronic Structure," Kevin R. Kittilstved

Chemistry Clubs

The **UMass Chemistry Club** has recently been exploring the chemistry of clay and glazes. With Professor Justin Fermann, club members learned to create pottery on pottery wheels and about the processes the clay undergoes when firing in the kiln. The club then created their own ceramic glazes from transition metal compounds and based off of the chemistry of the transition metal ions present, also predicted what they would look like after being fired once more. UMass Chemistry Club focuses on events that help people get excited about chemistry. From "just for fun" activities to planning more outreach events, this club envisions doing countless other projects – from brewing apple cider to blacksmithing – in the near future.

The ACS Club at UMass is a student-run chapter of the American Chemical Society that was brought to UMass in 2015. The club holds many social and networking events where students can get to know other chemistry majors as well as learn to navigate the professional world. The ACS Club partnered with the Chemistry Club during homecoming weekend to provide fun, hands-on, scientific demonstrations for families ranging from creating micelles in milk to lighting up the room with luminol. The two clubs also held frequent pottery nights, shaping their own clay creations, and learning about the chemistry of glazes.

During regular club meetings, UMass professors are invited to give short talks to familiarize members with the faculty and their amazing research. In addition, many meetings are devoted to student-run panels on joining research labs, picking classes, and writing cover letters or resumes. With fundraising, the club sent some members to the ACS national meeting in New



iCONS by Cameron Holden, iCons Manager

We had another exciting year in the UMass iCons Program!

The UMass iCons Program (Integrated Concentration in Science) recruits students across 25 science and engineering majors to identify global problems and find cutting-edge solutions.

At the May 4th iCons Senior Celebration there was, in fact, much cause to celebrate. Not only did the fifth cohort of iCons students graduate from the program, but the



Michele Pugnaire, iCons Director Justin Fermann, Kurt Schultz, Dean Tricia Serio

first-ever iCons Alumni Award was presented. Kurt Schultz was the inaugural recipient of the Mahoney Alumni Award for the iCons Program. This award is the first of its kind to recognize iCons graduates who demonstrate their continued engagement with the program, as well as the application of the iCons skillset in their careers after graduation. Schultz received \$5,000 and a crystal trophy. The prize is named after brothers William, Richard, and Robert Mahoney who all re-

ceived their degrees in Chemistry from the University of Massachusetts Amherst and have become leaders in their own industries and served as high-level alumni advisers on campus. The program is grateful to the Mahoney Family for their support and vision.

Schultz reflected, "I will forever see the world through the lens of an iCons student. I have high expectations for myself going forward, and I have high expectations for all

those who graduate from the iCons program at UMass Amherst. May our combined efforts be for the benefit of all."

In addition, we celebrated our fifth cohort of graduates, "The Fifth Element", as they marked the end of their time at UMass. We are so proud of them and wish them well as they en-



ter graduate school and the workforce imbued with the iCons mission and mindset. Here are some of their reflections on what they are taking with them:

"The most important skillset I have obtained from the iCons program was the iCons attitude and approach to tackling problems. This excited, independent yet collaborative mindset is at the end of the day what carries your research." (J. Lenef, Chemistry)

"The perspective I've gained from iCons has not only been a technical one in the sense I've been exposed to so many new societal problems, modes of scientific inquiry, methods and procedures but also a societal one at heart. The efforts undertaken by the iCons program and my involvement in it have made me not just a better scientist and researcher, but a better human being." (K.O'Connell, Physics)

We are grateful to the Chemistry Department and its loyal alumni base for their support throughout the years. We could not have come this far without it and are looking forward to another year of providing this unique learning experience at UMass: training the next generation of leaders in science!

Seminar by Michelle Farkas, Seminar Chair

The 2017-18 UMass Amherst Department of Chemistry seminar series brought many outstanding scientists to our campus to share their insights and recent discoveries. These speakers included several distinguished members representing the diverse field of chemistry, and included several women at the forefront of it. In addition, we hosted an unprecedented four of our own Assistant Professors as part of our fall pre-tenure line-up: Prof. Trisha Andrew, Prof. Min Chen, Prof. Kevin Kittilstved, and Prof. Eric Strieter.

We were also thrilled to host **Professor JoAnne Stubbe** from MIT for the William E. Mahoney Annual Lecture in October. Prof. Stubbe is a leader in the field of biochemistry, elucidating enzyme mechanisms, including ribonucleotide reductases, which play essential roles in DNA replication and repair. She has been the recipient of numerous awards including membership in the National Academy of Sciences, fellowship in the American Academy of Arts and Sciences, the Welch Award in Chemistry, and the National Medal of Science.

In November, **Professor Karen Wooley** from Texas A&M University presented the Stein-Covestro Honorary Seminar in Polymer Chemistry. Prof. Wooley is an internationally recognized leader in polymer chemistry, whose work has focused on the combination of organic syntheses, polymerization strategies, and polymer modification reactions to create unique, functional systems. Among others, she is a fellow of the American Academy of Arts & Sciences and the Royal Society of Chemistry, and has received the Royal Society of Chemistry Centenary Prize and the ACS Award in Polymer Chemistry.

Professor Eric Jacobsen from Harvard University was the Marvin D. Rausch Lecturer in Organometallic Chemistry this year. Prof. Jacobsen is a distinguished scientist in the fields of catalysis and organic chemistry, specifically focusing on the discovery and analysis of useful catalytic reactions, many of which have found widespread application in industry and academia. He has been honored with numerous awards including the Noyori Prize, the ACS H. C. Brown Award for Synthetic Methods, and the Remsen Award, and is a member of the National Academy of Sciences and the American Academy of Arts & Sciences. The Third Annual Graduate Student-Hosted Seminar in Chemistry was presented by Scott Anderson from the University of Utah, whose work focuses on nanoscale surface chemistry and has recently won the ACS Physical Division Award in Experimental Physical Chemistry.

Also, a highlight of each year's seminar program, UMass Amherst, Smith, Mt. Holyoke, Amherst, and Hampshire co-host the 5-College Lecture Series in Chemistry. For Spring 2018, UMass had the pleasure of hosting, which only happens once every five years! We welcomed **Professor James Wells** from the Department of Pharmaceutical Chemistry at the University of California, San Francisco as the 5-College Lecturer. Prof. Wells has had a distinguished career in both industry (at Genentech and as a founder of Sunesis Pharmaceuticals) and academia. His work focuses on understanding and modulating signaling processes in human cells through protein and small molecule design, with a focus on the inter-protein circuitry of pathways involved in cell death and inflammation. Prof. Wells is a member of the American Academy of Arts & Sciences and the National Academy of Sciences, and has received an array of awards and honorary lectureships.

In addition to the 'named' seminar speakers, the department had many luminaries within the field of chemistry participate in our seminar program in 2017-18, including Prof. Charles Brooks III (U. Michigan), Prof. Alexander Deiters (U. Pittsburgh), Prof. Tarun Kapoor (Rockefeller University), Prof. Yamuna Krishnan (U. Chicago), Prof. William Tisdale (MIT), and Prof. J. D. Tovar (Johns Hopkins University). 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 upcoming seminars and events can be found at www.chem.umass.edu/events-seminars/. We look forward to another exciting seminar series next year!



Professors Michelle Farkas, Richard Vachet, JoAnne Stubbe, Robert Mahoney



Professors Richard Vachet, Karen Wooley, Richard Stein, Don Wardius (Covestro)



Professors Michelle Farkas, Richard Vachet, Eric Jacobsen, and Jane Rausch



Professors Jeanne Hardy, James Wells, and Richard Vachet

Undergraduate Awards

Last Spring, on May 2, 2017, we held the annual Senior and Awards Dinner in the Amherst Room at the Campus Center. Over a hundred students, parents, faculty and staff joined to recognize the hard work and dedication of our 44 graduating seniors and to honor our students who have proven themselves to be among the very best this Universi-

ty has to offer. Many students were recognized for their exceptional achievements and 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. 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.



Dean Steve Goodwin congratulating the seniors and awardees

Academic Awards

CRC Freshman Chemistry Awards

Damon Schneider

Alexander Chau

Theodore Kottke

Gabrielle Farulla-Bastian

Robert Maxwell Williams Memorial Scholarships

Abigail Greenslade

Michael Clancy

Zoe Geannopoulos

American Chemical Society Analytical Chemistry Award

Dominique Carey

Rowell Scholarship and the Undergraduate Physical **Chemistry Award**

Julia Lenef

Royal Society of Chemistry Certificate of Excellence Award

Nicholas Russo

Edward Shapiro Scholarships

Marina Franc

Anton El Khoury

Alexandra Sahagian

Brett Whitchurch

Jessica Zebracki

Jay A. Pirog Scholarship

Megan Crane

John A. Chandler Memorial Scholarship

Marzbed Margossian

George R. Richason, Jr. Memorial Scholarship

Erin Phillips

American Chemical Society Hach Scholarships

Zachary Kirsch

Peter Antonucci

Research Awards

Oliver Zajicek Memorial Scholarship Awards

Anton El Khoury (Kaltashov group)

American Chemical Society Inorganic Chemistry Award

Alexandra Barbato (Knapp group)

American Chemical Society Organic Chemistry Award

Steve Capo (Venkataraman group)

Hypercube Scholar Award

Matthew Gentry (Metz group)

Uche Anyanwu Memorial Awards for Outstanding

Research 2017

Alexandra Barbato (Knapp group)

Gisele Andree (M. Chen group)

Mark Leon-Duque (You group)

Mr. Tompkins Award

Alexandra Barbato (Knapp group)

Undergraduate Research Award

Jem Sibbick (Tyson group)

Bates Research Fellowship

Duy Nguyen (Dubin group)

Bradspies Research Fellowship

Casey O'Brien (You group)

Professor Jack Ragle Research Fellowship

Haote Li (Venkataraman group)

Departmental Awards

Distinguished Undergraduate Instructor Award in Honor of Earl J. McWhorter and George R. Richason, Jr.

Scott M. Auerbach

Distinguished Graduate Teaching Assistant Award

in Honor of George R. Richason, Jr.

Banyuhay Serrano

Distinguished Undergraduate Teaching Assistant Award

in Honor of George R. Richason, Jr. David Kouvchinov

Positron Award

Jacob Adelman

American Chemical Society Membership Awards

Matthew (Donnie) Rollings

Gisele Andree

Connecticut Valley Section of

the American Chemical Society Student Award

Alexandra Barbato

American Institute of Chemists Award

Jacob Adelman

Departmental Recognition Awards

Bailey Ingalls

Nathaneal Park

Richard W. Fessenden Awards

Steve Capo

Alexandra Barbato

Senior Class Award

Alexandra Barbato



















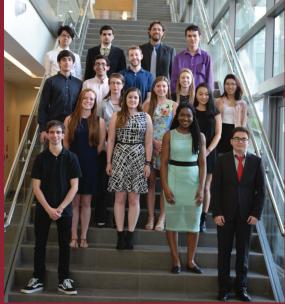
Chemistry Seniors 2017

May 2017 Jacob Adelman Sarmad Al-Khamees Alexandra Barbato Christopher Boussy Emily Boyle Steven Capo Anton El Khoury Aidan Finnerty Ross Furash Matthew Gentry Ho S Han Bailey Ingalls Ulrich Kakou Nicole Kirby Samantha Kriksceonaitis Jessica Maat Thanh Mai Carolyn Palmer

Nathaneal Park Marguerite Rushanan Kanae Sasaki Gabriel Teso Connie Yoon Jessica Zebracki

Summer 2017 Nicholas Caldarone Sang Kim David Kouvchinov Yina Li Abigail Lynn Duy Nguyen

Fall 2017 Aline Mweze







Undergraduate Awards

The twentieth(!) annual Senior and Awards Dinner was held at the Campus Center on April 13, 2018. More than a hundred students, parents, faculty and staff attended the event, which recognized our graduating seniors and students who have distinguished themselves in the pursuit of academic excellence. Following a buffet dinner, 40 awards were presented to 31 deserving undergraduates. The graduating seniors were welcomed with a rousing ovation. We thank our outstanding students for their contributions to the department, and thank the many generous donors who make these awards possible.



Giselle Andree accepting the Jack Ragle Research Fellowship from Prof. Michael Knapp



Prof. Richard Vachet, Sara Chedid. winner of the John A. Chandler Memorial Scholarship, and Joann Chandler

Academic Awards

CRC Freshman Chemistry Awards

Justin Baker

Tiernan Kennedy

Casey Phillips

Jeremy Quercia

Robert Maxwell Williams Memorial Scholarships

Gabrielle Farulla-Bastian

Maura Haley

Yiwen Xie

American Chemical Society Analytical Chemistry Award

Thomas Kumlin

Royal Society of Chemistry Certificate of Excellence Award

Tiernan Kennedy

Edward Shapiro Scholarships

Lucas Ghilardi

Cameron Kaminsky

Jennie Paik

Alexandra Sahagian

Yuying Zhang

Jay A. Pirog Scholarship

Lynh Le

John A. Chandler Memorial Scholarship

Sara Chedid

George R. Richason, Jr. Memorial Scholarship

Mark Anthony Leon-Duque

Thomas R. "Casey" Stengle Scholarship

Sarah Brown

American Chemical Society Hach Scholarships

Gisele Andree

Kareem Mohamed-Aly

Research Awards

Oliver Zajicek Memorial Scholarship Award

Gisele Andree (M. Chen group)

American Chemical Society Inorganic Chemistry Award

Christopher Roy (Kittilstved group)

American Chemical Society Organic Chemistry Award

Julia Lenef (Venkataraman group)

American Chemical Society Physical Chemistry Award

Gisele Andree (M. Chen group)

Mr. Tompkins Award

Matthew (Donnie) Rollings (Venkataraman group)

Undergraduate Research Award

Matthew (Donnie) Rollings (Venkataraman group)

Bradspies Research Fellowship

Mark Anthony Leon-Duque (You group)

Professor Jack Ragle Research Fellowship

Gisele Andree (M. Chen group)

Tarselli Family Research Award

Isabella Jaen Maisonet (Knapp group)

Departmental Awards

Distinguished Undergraduate Instructor Award in Honor of Earl J. McWhorter and George R. Richason, Jr.

Christopher McDaniel

Distinguished Graduate Teaching Assistant Award

in Honor of George R. Richason, Jr.

Michael Mingroni

Distinguished Undergraduate Teaching Assistant

Award in Honor of George R. Richason, Jr.

Katherine Poisson

Positron Award

Katrina Nguyen

American Chemical Society Membership Awards

Zachary Kirsch

Jem Sibbick

Connecticut Valley Section of the American Chemical

Society Student Award

Julia Lenef

American Institute of Chemists Award

Katherine Poisson

Departmental Recognition Awards

Katrina Nguyen

Casey O'Brien

Richard W. Fessenden Awards

Marzbed Margossian

Casey O'Brien

Senior Class Award

Matthew (Donnie) Rollings



Chemistry Seniors 2018

May 2018 Antony Abi-Elias Rashad Almadani Peter Antonucci Justin Campbell Abigail Candee Megan Crane Luis Cristian Thomas Drews Ethan Dunleavy Marina Franc Spencer Keoppel

Zachary Kirsch Julia Lenef Haote Li Slawomir Madro **Emily Mai** Daniel Marco Alexandra McEnroe James Millet Patrick Moquin Aidan Murphy Katrina Nguyen Casey O'Brien Jennie Paik Eyasha Pandey Erin Phillips Katherine Poisson Matthew (Donnie) Rollings

Jem Sibbick
Jeffrey Tsai
Justin Vadenais
Andras Watzker
Cooper Wharton
Fall 2018
Marzbed Margossia

Christopher Roy

Nicholas Russo

Zachary Schafer

Allyson Shea

Fall 2018 Marzbed Margossian Tudor Muntean Julie Novelli Alexander Santoro













The summer timeline for the Goessmann Gazette has allowed us to include recent graduates from 2018. The Chemistry Department celebrated the achievements of its seniors with parents, faculty and staff at the Senior & Awards Dinner and the Senior Reception. The reception was held in the Integrated Sciences Building just prior to the College of Natural Sciences Senior Celebration at the Mullins Center on Saturday, May 12th. The Undergraduate Commencement Ceremony was Friday, May 11th.









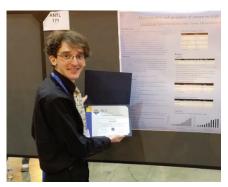




undergraduate Research Projects

Determination and Speciation of Arsenic in Single Rice Grains by Jem Sibbick

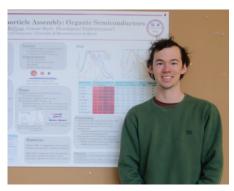
In many parts of the world, the issue of environmental arsenic contamination has been a cause of concern for scientists for some time. The presence of arsenic in water supplies and foodstuffs such as rice has the potential to increase rates of cancer and heart diseases for large populations. Due to its particular biochemistry, the rice plant is adept at absorbing arsenic from the soil. Rice is one of the most commonly consumed foods on earth; as such, many methods have been developed in the analytical community to perform arsenic determination and spe-



ciation analysis in rice. Most groups will do this by taking a large sample of rice consisting of many grains and grinding the sample into powder. It is typically assumed that the rice grains are homogeneous—that all rice grains have a similar concentra-

tion of arsenic. Working with Professor Julian Tyson, I tested this assumption by developing a validated method of arsenic determination and speciation in single rice grains using hydride-generation atomic fluorescence spectrometry. My research indicates that the assumption of homogeneity is not as valid as previously assumed, with total and inorganic arsenic levels demonstrating wide variation between single grains, from a factor-of-two up to a factor-of-five difference.

Nanoparticle Assembly: Organic Semiconductors by Matthew (Donnie) Rollings



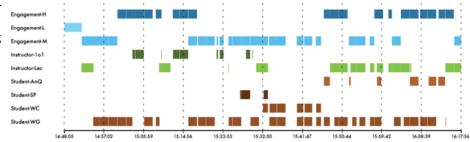
My research in the Venkataraman (DV) lab focuses on improving organic electronic materials. I use didodecyl perylene diimide (PDI), a semiconductor molecule that can be used in electronic devices like solar cells and

thermoelectrics. These devices often demonstrate improved performance and consistency when made using nanoparticles instead of from bulk solution. I make PDI into nanoparticles and try to change their structure by varying the surfactant, a crucial component of nanoparticle synthesis. We think that the interaction between the side chains of the surfactant and PDI directs aggregation as the droplets crystallize. I measure the UV-Vis absorption and photoluminescence spectra of the nanoparticles and classify the results using a theory of aggregation developed by Prof. Frank Spano at Temple University. The type of aggregation influences the optoelectronic properties of the material; determining the surfactant effect on aggregation could therefore make available a new 'knob' to turn to achieve just the right device characteristics, starting at the material level. All nanoparticles were found to have significantly altered spectral features from the isolated PDI dissolved in chloroform. Nanoparticles made from differing surfactants did demonstrate unique spectral profiles, although the differences were more subtle and a relationship has not yet been determined. To aid in this process, the PDI side chain will be varied to provide a second axis of comparison.

Evaluation of Flipped Format Method in General Chemistry Courses by Eyasha Pandey

Believe it or not, not all chemistry research is done in a lab! This past semester, I worked with Professor Gabriela Weaver to determine the effectiveness of a flipped-classroom vs. a traditional lecture-based format. A flipped-classroom format consists of students watching the lecture on their own time and meeting with the professor once or twice a week for a 90-minute problem solving session. In these sessions, students are broken up into groups and presented with problems that utilize the material that was taught in the online lectures. There is a five minute quiz to ensure students watched the lecture, followed by a short recap of the main concepts. Then, the groups are left to work together, with teaching assistants and the professor walking around to answer any questions. At the end of the session, the problem set is reviewed by groups presenting their solutions to the whole group. This format has been

implemented at Purdue University where Professor Weaver used to teach. I have been analyzing the recordings of these sessions and determining the optimal way to run them. Many factors are considered, like how time is broken up, whether the whole group is engaged, and what kinds of problems to present. The flipped-classroom format for general chemistry courses has proven to be more effective than lecture-based and in the coming years we hope to implement flipped classrooms in more chemistry courses.



A common chart, using the Generalized Observation and Reflection Platform from the University of California Davis, displays the activity of students as a session goes on. The y-axis represents multiple categories while the x-axis shows time.

Instrumental Analysis Research Projects

by Ruthanne Paradise, Director of Analytical & Physical Laboratories

Each fall, undergraduate and graduate students take Instrumental Analysis. It is a unique course because it pairs a lecture about the theory of instrumentation with a lab that allows them to develop their own analytical methodologies during an independent research project. The students are often met with a mixture of success and failure as they work on their projects.

This year students pursued six different projects. Four groups focused on their own interests related to contaminants in the environment, one group worked with Prof. Hans Mentzen to analyze hops, and another worked with Prof. Ruthanne Paradise to analyze hormones. To give you an idea of how different the projects are, here are the titles:

"Motor Oil and Hydrocarbons as Potential Crop Pollutants," James Millet, Jennie Paik, Donnie Rollings

"Arsenic and Lead Detection in Water Sources on UMass Campus Using GFAAS," Patrick Moquin; Antony Abi-Elias, Oladele Amos Oluwaviose

"Study of Nitrite and Nitrate in the Mill River System," Marina Franc, Casey O'Brien and Chris Roy

"Determination of Lead Concentration in Amherst-area Water Supply Using Flame Atomic Absorption," Zack Kirsch, Eyasha Pandey, Jem Sibbick

"Identification and Quantification of Aroma-Contributing Compounds in Hops," Katherine Poisson, Zachary Schafer, Cooper Wharton

"Differentiation and Quantification of Hormones and Neurotransmitters for Breath Analysis using Liquid Chromatography-Mass Spectrometry," Thomas Drews, Slawomir Madro, Justin Vadenais, Sicheng Xiong

Students may not have proved or disproved their hypotheses, but they all honed their skills in reading literature, developing methodologies for analysis, and persevering in the face of the many unexpected turns research can take. One exciting byproduct of the research done by the group analyzing hops is that their work will be developed and serve as a springboard for a new training experiment for Instrumental Analysis this fall, and potentially the Quantitative Analysis course, as well!

Collaborative Undergraduate Research in Energy (CURE) Program Summer 2018

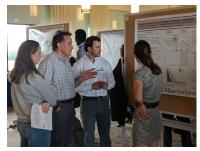
by Ruthanne Paradise

Each summer, the Chemistry department hosts up to ten students to carry out research for ten weeks. They come to campus as participants in the Collaborative Undergraduate Research in Energy-Research Experience for Undergraduates (CURE-REU) NSF grant. This program was initially started in 2007 and led by Prof. S. "Thai" Thayumanavan and Prof. Justin Fermann. Over the years, the leadership transitioned over to Prof. Fermann and then last year Prof. Kevin Kittilstved and Prof. Ruthanne Paradise have taken the reins to guide these students through a summer of research. Prof. Kittilstved is in charge of coordinating the research and Prof. Paradise directs the educational portion of the program and has carried out the majority of the administrative duties.



This year we had a full cohort of ten students. They carried out collaborative research, with pairs of participants working in two different labs. Their projects are related to each other because they are working on two different aspects of the same problem. To demonstrate this relation to others, they present a joint poster to the public at the end of their ten weeks at UMass.

All in all, this summer was a great success. Students learned more about what kind of research they like to participate in, as well as all sorts of new skills from programming languages to running protein purification gels. One student even decided they would like to go on to graduate school because they found the experience that enriching. We look forward to meeting next summer's students.





Classroom Laboratories by Ruthanne Paradise and Bill Schmitt

The physical/analytical labs are presently upgrading several instrument platforms with state of the art instruments, purchased with newly acquired funds that came from student lab fees.

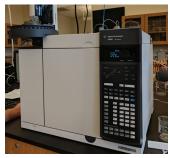
This summer, we replaced our last three functioning Cecil 2041 spectrophotometers with sixteen Vernier Vis spectrophotometers: one for each lab pair in Honors General Chemistry. These will provide direct hands-on measuring and recording of experimental data into recently purchased lab notebook computers.

Vernier wireless pH measuring probes were purchased that permit direct measuring and recording of data onto student PC notebooks. The systems will replace 20 aging PASCO pH meters.

After 20 years of service, the Agilent 6890 teaching gas chromatograph has been retired, and replaced with a state-of-the-art Agilent 7890 gas chromatograph. Improvements in speed and turn-around time mean that students will get more out of each lab. We are planning additional upgrades to the teaching labs which will take place in the summer and fall of 2018.







Vernier Vis spectrophotometer

Staff Notes

Raina Kittilstved has been hired into the new Organic Chemistry Lab Supervisor position. Manju Sharma has been hired into the Organic Chemistry Lab Manager position replacing Raina, after Manju's many years of research in the Maroney and Knapp research labs.

The Assistant to the Head position is now held by **Rebecca David**. **Tania Wellen** is our new Seminar and Alumni Programs Coordinator. **Amy Golenski** has been hired as our new Bookkeeping Assistant/Procard Records Manager. **Susan Stinson** is now the administrative assistant for both the Chemistry-Biology Interface (CBI) and UMass Biotech Training (BTP) programs. **Lorraine Cox** has joined the undergraduate program as a part-time assistant in ISB.

Nikki Tebaldi Serves on the CNS Staff Advisory Committee

The Dean of the College of Natural Sciences, Tricia Serio, has formed a Staff Advisory Committee, which has been working towards defining a mission, determining goals, and planning staff events. The Department of Chemistry's committee member is Nikki Tebaldi, a member of the BMB & Chemistry IT team.

The current mission of the committee is to support all staff in the College by serving as a conduit for information, acting in an advocacy role, and recognizing staff achievements. A main goal of the committee is to empower employees within the College of Natural Sciences, enhance their workplace quality, and build a sense of community.

John Maher Wins CNS Outstanding Staff Award

John Maher is a Systems and Networking Administrator with the joint Chemistry and Biochemistry and Molecular Biology IT group who has worked behind the scenes to set up the fundamental infrastructure that shapes how we do things technologically, and to make sure that it all works smoothly. He was instrumental in setting up the shared Chemistry and BMB network which is used by "everybody"—staff, faculty, research labs, and students—for sharing files and printers, archiving data, etc. He also set up the LDAP directory system used to access the departmental wireless, file servers, Wordpress sites, meeting room booking, and a million other useful things. The CNS Outstanding Staff Award is given to 1-3 people each year and recognizes the crucial role played by staff members in facilitating the success of the College of Natural Sciences. Congratulations to John!

Lisa Korpiewski Holds New Position in IALS

Lisa Korpiewski, Web page/publications designer in the Chemistry department for many years, has transitioned into a new role as a full-time Website and Graphic Designer for the Institute for Applied Life Sciences (IALS). For about a year, Lisa split her time between Chemistry and IALS, and last October she began working solely for IALS. Many Chemistry faculty are members of IALS, so Lisa stilll has connections to our department.

In addition to setting up and managing the department website, Lisa was responsible for production, design and photography for the Goessmann Gazette. We are thankful for all her help and pleased we still interact with her.

Memoriam

Howard Stidham

Professor Howard Stidham passed away on November 13, 2017 at the age of 92. Howard graduated from Manchester High School in Manchester, Connecticut in 1943. He enlisted in the U. S. Army shortly thereafter, serving two terms, from 1943 to 1945 in Germany and from 1945 to 1947 in The Philippines. He then attended Trinity College, receiving his B.S. in 1950,



and in 1955 he received a PhD in chemistry from MIT. After a year as Chief Spectroscopist at Dewey and Almy Chemical Company, he joined the chemistry faculty at UMass Amherst in 1956. Howard educated countless students during his 61-year career at UMass Amherst. Among his contributions, he was particularly known for teaching the Physical Chemistry Lab for several decades. He also regularly taught graduate courses in Statistical Mechanics and very recently wrote a textbook, "Statistical Thermodynamics for Beginners." Howard was an experimental physical chemist who used IR and Raman spectroscopy to explore the properties of polymers and flexible molecules, particularly their stable configurations and how these depend on the phase (gas/liquid/solid). He was a rigorous scientist (with a wry sense of humor!) who taught spectroscopy to a great many graduate and undergraduate students, both in his own lab and in several other research groups in Chemistry and Polymer Science and Engineering (PSE). Howard published over 80 papers, much of this work involving collaborations with other research groups both on and off campus, particularly those of James Durig (U. South Carolina) and Shaw L. Hsu (PSE).

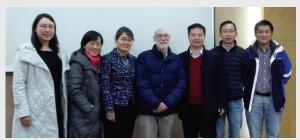
Michael Bruno

Mike Bruno was born on October 17, 1933 in Springfield, Massachusetts, and grew up in Springfield. He was a Chemistry major at UMass Amherst, earning his Bachelor's degree in 1955. After graduating from UMass, Mike served in the Army and earned a Ph.D. in Organic Chemistry from Cornell University. He worked at DuPont for many years, starting as a Research Chemist and advancing to Plant Superintendent. During this period, he filed many of the fundamental process patents on DuPont film products. Starting in 1973, he worked for Raychem Corp in Menlo Park in a variety of managerial positions. He and his wife, Marge, raised their two children in Los Altos, California, where Marge served as Mayor for many years. Mike passed away on March 31, 2017, following a battle with pancreatic cancer.

In 2014, Mike and Marge established the Michael Bruno Chemistry Scholarship in order to create educational opportunities for students who would otherwise have none. It provides financial support to a Chemistry undergraduate with demonstrated financial need and a GPA of at least 3.0, with preference given to a resident of Massachusetts.

Paul Dubin

Professor Paul L. Dubin passed away on May 23, 2018 at the age of 77. Prof. Dubin joined the UMass-Amherst faculty over a decade ago after a long and fruitful career in industry (Dynapol, Memorex Corporation and Clairol Research Laboratories) and academia (twenty-four years on faculty at the Chemistry Department at Indiana-Purdue University). Prof. Dubin has made a lasting contribution to the field of physical chemistry publishing nearly 200 peer-reviewed papers. These papers have been cited nearly 10,000 times. Prof. Dubin was very active in building bridges not only among scientists from different countries (it is not an exaggeration to say that the geography of his collaborations spans the entire globe), but also among disciplines. As one of the leading figures in colloidal chemistry, he actively engaged with both biologists and physicists, firmly believing that further advancements in the life sciences are impossible without incorporation of physical chemistry into biological research. One of his most important scientific accomplishments is the meticulous study of complex coacervation (a unique type of electrostatically-driven liquidliquid phase separation, resulting from association of oppositely charged macro-ions) in colloidal and biological systems. Prof. Dubin also made very important contributions to both theory and practice of liquid chromatography and electrophoresis, which included editing a highly influential book Aqueous Size Exclusion Chromatography and several patents. However, Prof. Dubin's most important (and certainly most loved) "accomplishments" are his former students. Over 30 graduate students received advanced degrees under his tutelage, and now work in government laboratories, industry and academia both across the country and across the continents (including Chemistry professors in Michigan, Turkey and China).



Shanghai Reunion 2017. Paul Dubin with former postdocs Yaxun Fan, Yajuan Li, Yilin Wang, Xuhong Guo, Yunfeng Yan, Yisheng Xu

Jacek Lubinkowski

Dr. Jacek Lubinkowski (PhD, 1973) passed away Dec 28, 2017, in Caracas, Venezuela, at the age of 71. Born in Edinburgh, Scotland to Polish parents who had taken part in the Resistance, the family soon emigrated to Springfield, MA, where Jacek grew up. Jacek received his BS from the University of Rochester before coming to UMass Amherst, where he did his doctoral research with Prof. William McEwen. He enjoyed a very distinguished career, teaching Organic Chemistry at the Universidad Simón Bolívar in Caracas, carrying out research with Venezuela's oil ministry Intavep S.A., and continuing to collaborate with Prof. McEwen on various projects.

Alumni

Annual Mahoney Life Sciences Prize Established for CNS Faculty

The Mahoney Life Sciences Prize, an annual competition for CNS scientists engaged in high-impact applied life sciences research, is made possible through the generosity of the Mahoney family to recognize UMass Amherst scientists whose work significantly advances connections between research and industry.

The prize is awarded to one faculty member who is the principal author of a peer-reviewed paper about original research on any topic in the life sciences that focuses on new research with translatable applications to industry and society. It is the first faculty paper prize for CNS, and includes an award of \$10,000 as well as opportunities to present the research to industry leaders and the UMass Amherst community.

The three Mahoney brothers – Robert, Richard and William - received their degrees in chemistry from UMass Amherst. They went on to become leaders in their own industries and have served as high-level alumni advisers to the campus.



The inaugural prize winner is chemistry's own Jeanne Hardy for research focusing on a key protein linked to neurological disorders.

Robert Mahoney '70, Richard Mahoney '55, '83Hon, Jeanne Hardy, William Mahoney '55, Chancellor Kumble R. Subbaswamy, and Tricia Serio, Dean, CNS

Annual Mahoney Alumni Award Established for iCons Program Graduates



The College of Natural Sciences (CNS) announced the establishment of the Mahoney Alumni Award for the iCons Program, an Concentration annual award to be bestowed to one alumna or alumnus

of the Integrated Concentration in Science (iCons) Program who demonstrates application of the attitudes, knowledge, and skills developed in the program and who has shown engagement and support of the iCons community since graduation.

Mahoney and Lee article/photo credit: Office of News and Media Relations

Gift to UMass Amherst Expands Opportunities for Underrepresented and First-Generation Students in Sciences

A new program created with a gift from University of Massachusetts Amherst alumnus William "Bill" A. Lee, executive vice president of research at Gilead Sciences, will broaden opportunities for underrepresented and first-generation UMass Amherst students who aspire to be scientists.



The new William Lee Science Impact Program (Lee-SIP) at the College of Natural Sciences gives selected undergraduates the opportunity to work with faculty on a wide range of research projects. Currently, 13.4 percent of the college's 6,067 undergraduates are

from underrepresented groups, and 29 percent are firstgeneration college students.

Lee-SIP Scholars will be directly mentored by faculty, work within a research team, and participate in professional development workshops. These activities are intended to prepare participants for a wide range of science-based careers. As a result of participating in this program, students will be able to use principles of the scientific method to develop a research proposal, evaluate scientific data in their respective field, formulate conclusions and effectively communicate scientific findings to experts and general audiences. Selected applicants will be awarded fellowships that include stipends, funding for research supplies and an allowance for living expenses.

"Bill's generosity will provide an unprecedented opportunity for our students, particularly those who are the first in their families to attend college, to engage in an independent research project," says Tricia Serio, dean of the College of Natural Sciences at UMass Amherst. "This gift has the power to transform students' success and career opportunities. I am so excited for them and grateful to Bill for supporting this program."

Lee, who earned a BS in chemistry from UMass Amherst in 1977, was the first in his family to graduate from college, where he developed an understanding of the impact research can have on both students and society. "When Dr. Marvin Rausch asked me if I was interested in working in his lab over the summer, I had no idea of what to expect or how it would change my course in life. I thrived on the comradery with grad students and postdocs in the lab and for the first time, science left the text book and became alive."

Lee went on to earn a PhD in chemistry at the University of California, San Diego, and conducted postdoctoral studies at the Ecole Polytech Federal Lausanne in Switzerland and the University of California, Santa Barbara.

He joined Gilead Sciences in 1991 as director, pharmaceutical product development. In 2015, he was appointed executive vice president, research and has been responsible for the expansion of the company's research and preclinical activities across a range

of therapeutic areas, including HIV, liver diseases, hematology and oncology, inflammation and respiratory diseases and cardiovascular conditions. Prior to joining Gilead, Lee was head of drug delivery at California Biotechnology, Inc. and began his career as a research scientist at Syntex Research in Palo Alto, California. During his career, he led discovery efforts and the advancement of new drugs that changed the course of many chronic diseases, including transplantation, HIV, hepatitis B and hepatitis C.

UMass is a Family Affair By Michael Tarselli '03

Editor's Note: Mike Tarselli (BA, Chemistry, cum laude, UMass, 2003; PhD, Chemistry, Univ. of North Carolina-Chapel Hill, 2008) is an Associate Director in Chemistry Information Systems at the Novartis Institutes for BioMedical Research. He shares his thoughts on his undergraduate experience and the newly established Tarselli Family Research Award, which supports summer research for rising juniors who plan to pursue research careers in the biotech and pharmaceutical fields.



I have a longstanding love for UMass Amherst. I first visited campus at the tender age of five; we took the library elevator all the way up to 24, and I can remember the view to this day. Of course, there's a few more buildings now than there were in 1986!

Furthermore, it's a family affair – two uncles, my brother, my sister-in-law, my best friend, and many of my cousins came here for school. Most were (and are today) scientists and engineers.

When I first came to UMass, I was a Pre-Med without much direction. I didn't feel a strong pull in my intro Bio or Psych classes. I first lit up, as many chemists do, in Prof. Dave Adams' sophomore organic ("orgo") class. That's when I realized chemistry could be both a passion and a career.

I was lucky that, at the time, an Adjunct Professor, Dr. Tomi Sawyer, was offering internships for sophomores and juniors who wanted to work in pharmaceutical chemistry. Without exaggeration, I would not have gone for my PhD or into medical research without that experience.

My family and I established this scholarship to help other students who share my interests to choose chemistry, especially if, like me, they're at an inflection point in their college life story. Hopefully, recipients will see the passion I have for both UMass and chemistry, and give back when they're able.

I'd also like to comment that age or gift amount should not stop people from giving back. Anything helps! I wanted to start small and watch something grow, instead of waiting to give more later in my career.



Prof. Mike Knapp and Mike Tarselli presenting Isabella Jaen Maisonet with the Tarselli award and personalized lab coat.

Inaugural Recipient of the Tarselli Family Award

Isabella Jaen Maisonet, rising junior chemistry major, is the first recipient of the Tarselli Family Award. Isabella writes, "With the Tarselli Family Grant, I will be continuing my research into the Fe²⁺ α-ketoglutarate-dependent oxygenase, Factor Inhibiting Hypoxia Inducible Factor (FIH) and its selectivity for certain peptides. I will be investigating the steady-state kinetics of ARD hydroxylation by FIH, using ARD peptides which have been mutated to express different amino acids at the target residue sites. Because of the generous scholarship from Mike Tarselli, I have raised my own expectations and goals scientifically as well as my personal goals after graduation. His belief in "paying it forward" set the bar for excellence the moment I received the award and inspires me daily to work towards making an impact with my research. The Tarselli Family Grant has helped me see the scientific community as a collaborative space, where discovery and innovation are stemmed from inspiring passion in young scientists."

ENDOWMENTS

Roger G. Bates Chemistry Fund

Michael Bruno Chemistry Scholarship

J.F.B. Fund for Undergraduate Research in Chemistry

John A. Chandler Memorial Scholarship in Chemistry

Chemistry Undergraduate Research Scholarship

Richard Fessenden Fund

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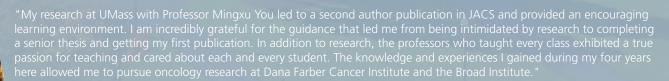
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Hardy Wins Inaugural Mahoney Life Sciences Prize

Professor Jeanne Hardy, whose research focuses on a key protein linked to neurological disorders such as Alzheimer's disease, has won the inaugural Mahoney Life Sciences Prize. Established by UMass Amherst Chemistry alumni Richard, Robert and William Mahoney, the \$10,000 prize recognizes scientists from the university's College of Natural Sciences whose work significantly advances connections between research and industry. The prize will be awarded annually to one faculty member who is the principal author of an exceptional peer-reviewed paper describing original research in the life sciences with translatable applications to industry and society.

"We had two purposes in establishing the Mahoney Life Sciences Prize," said Richard Mahoney, former president and CEO of Monsanto. "To let science-based companies see the extraordinary R&D being done in their field by UMass scientists and to show the UMass scientists that the corporate life sciences community places a high value on research that they can use to solve problems or provide future growth opportunities." After receiving their degrees in chemistry from UMass, Richard, Robert and William Mahoney went on to become leaders in their own industries and to serve as high-level alumni advisers to the campus.

Prof. Hardy's research paper, "Multiple proteolytic events in caspase-6 self-activation impacts conformations of discrete structural regions," was published in the *Proceedings of the National Academy of Sciences* in September 2017. A crystallographer and protein engineer who has developed tools and techniques for determining and modifying the structure and function of proteins, Hardy has for several years intensively investigated a group of proteins known as caspases. These "molecular scissors" cut up proteins and are active in programmed cell death and inflammation. In particular, one known as caspase-6 is associated with neurological disorders such as Alzheimer's and Huntington's diseases. Recently, Hardy called caspase-6 "an attractive molecular target for treatment of neurodegeneration," and her lab has been characterizing the structural details of caspase-6 activation and function.

In their most recent research, Hardy used a new approach to reveal "distinct conformational dynamics in critical regions of the caspase-6 structure" that had not been observable by any other techniques. As a result, they offer "two important new findings" that shed more light on caspase-6's mechanisms and note that the changes they describe "may inspire approaches for manipulating caspase-6 in the context of neurodegeneration." The new molecular details of caspase-6 dynamics "provide a comprehensive scaffold for strategic design of therapeutic approaches to neurodegenerative disorders." A panel of expert judges from the life sciences sector observed that the "biomedical implications are significant" and "this could turn out to be one of 'the' pivotal studies in the effort to combat Alzheimer's."